

Appendix C

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CHEMICAL SUMMARY FOR 1,3-DIETHYLTHIOUREA

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 1,3-diethylthiourea are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 1,3-DIETHYLTHIOUREA

Characteristic/Property	Data	Reference
CAS No.	105-55-5	Lide (1995)
Common Synonyms	N,N-diethylthiourea	Lide (1995)
Molecular Formula	C ₅ H ₁₂ N ₂ S	Lide (1995)
Chemical Structure	C ₂ H ₅ NHCSNHC ₂ H ₅	Lewis (1993)
Physical State	buff solid	Lewis (1993)
Molecular Weight	132.32	Lide (1995)
Melting Point	78 °C	Lide (1995)
Boiling Point	decomposes	Lide (1995)
Water Solubility	4.56 g/L	PHYSPROP (1998)
Density	1.11 mg/m ³	Ohm (1997)
Vapor Density (air = 1)	no data	
Koc	49 (estimated)	HSDB (1998)
Log Kow	0.57	PHYSPROP (1998)
Vapor Pressure	0.240 mm Hg at 25 °C (estimated)	PHYSPROP (1998)
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	6.9x10 ⁻⁸ atm m ³ /mole (estimated)	PHYSPROP (1998)
Fish Bioconcentration Constant	2 (estimated)	HSDB (1998)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into aquatic waters, 1,3-diethylthiourea is not expected to adsorb to suspended solids and sediments in water based upon an estimated Koc of 49 (HSDB, 1998; Swann et al., 1983), determined from a log Kow of 0.57 (Govers et al., 1986, as cited in PHYSPROP, 1998) and a regression-derived equation (Lyman et al., 1990).

Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990) based on an estimated Henry's Law constant of 6.9x10⁻⁸ atm-m³/mole (PHYSPROP, 1998; SRC, 1998). Since thiourea, a structurally similar compound, was found to be stable to hydrolysis and photolysis (Schmidt-Bleek et al., 1982, as cited in HSDB, 1998), 1,3-diethylthiourea is also expected to be stable to both hydrolysis and photolysis. According

to a classification scheme (Franke et al., 1994), an estimated BCF of 2 (HSDB, 1998; Lyman et al., 1990) suggests that the potential for bioconcentration in aquatic organisms is low.

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), 1,3-diethylthiourea, which has an estimated vapor pressure of 0.24 mm Hg at 25 °C (PHYSPROP, 1998; SRC, 1998), should exist solely as a vapor in the ambient atmosphere. The predominant removal process of 1,3-diethylthiourea from the atmosphere is reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 4 hours (Atkinson, 1988). 1,3-diethylthiourea, which has a high estimated water solubility of 4.56 g/L (PHYSPROP, 1998; SRC, 1998), is expected to adsorb onto atmospheric particulate material; the small amount of 1,3-diethylthiourea deposited onto particulate material may be physically removed by wet and dry deposition (HSDB, 1998).

C. Terrestrial Fate

Based on a classification scheme (Swann et al., 1983), an estimated Koc of 49 (HSDB, 1998), determined from a log Kow of 0.57 (Govers et al., 1986, as cited in PHYSPROP, 1998) and a regression-derived equation (Lyman et al., 1990), indicates that 1,3-diethylthiourea is expected to have very high mobility in soil. Volatilization of 1,3-diethylthiourea from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an estimated Henry's Law constant of 6.9×10^{-8} atm-m³/mole (PHYSPROP, 1998). In addition, 1,3-diethylthiourea is not expected to volatilize from dry soil given its estimated vapor pressure of 0.24 mm Hg (PHYSPROP, 1998; SRC, 1998).

D. Summary

If released to air, an estimated vapor pressure of 0.24 mm Hg at 25 °C indicates that 1,3-diethylthiourea should exist solely as a vapor in the ambient atmosphere. Gas-phase 1,3-diethylthiourea will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 4 hours. 1,3-Diethylthiourea is not expected to adsorb to suspended solids and sediments in water. An estimated BCF of 2 suggests the potential for bioconcentration in aquatic organisms is low. If released to soil, 1,3-diethylthiourea is expected to have very high mobility based upon an estimated Koc of 49, and, therefore, it has the potential to leach to groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon a Henry's Law constant of 6.9×10^{-8} atm-m³/mole. Volatilization from dry soil surfaces is not expected to occur based upon the vapor pressure of this compound.

SUMMARY FOR 1,4-BUTENEDIOL

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of 1,4-butenediol are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF 1,4-BUTENEDIOL

Characteristic/Property	Data	Reference
CAS No.	110-64-5	Grafje et al. (1985)
Common Synonyms	2-butene-1,4-diol (mixed isomers)	Grafje et al. (1985)
Molecular Formula	C ₄ H ₈ O ₂	Grafje et al. (1985)
Chemical Structure	HOCH ₂ CH=CHCH ₂ OH	Grafje et al. (1985)
Physical State	pale, yellow liquid	Grafje et al. (1985)
Molecular Weight	88.1	Grafje et al. (1985)
Melting Point	4 °C (cis); 25 °C (trans)	Howard and Meylan (1997)
Boiling Point	235 °C (cis); 135 °C @ 12 mm Hg (trans)	Howard and Meylan (1997)
Water Solubility	soluble; estimated to be >1x10 ³ g/l	Grafje et al. (1985); SRC (1998)
Density	specific gravity = 1.07 @ 25 °C (liquid)	Weiss (1986)
Vapor Density (air = 1)	no data	
Koc	8.6 (estimated)	Lyman et al. (1990)
Log Kow	-0.81	Hansch et al. (1995)
Vapor Pressure	4.7x10 ⁻³ mm Hg @ 25 °C (extrapolated)	Grafje et al. (1985)
Reactivity	no data	
Flammability	not flammable: flash point >100 °F	Cote (1997)
Flash Point	263 °F (Cleveland open cup)	Flick (1991)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	1.54x10 ⁻¹⁰ atm m ³ /mole (estimated)	Meylan and Howard (1991)
Fish Bioconcentration Constant	0.14 (estimated)	Boethling et al. (1994)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

An estimated Koc of 8.6, determined from a log Kow of -0.81 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990), indicates that 1,4-butenediol is not expected to adsorb to suspended solids and sediment in water. Also, an estimated Henry's Law constant of 1.54x10⁻¹⁰ atm m³/mole at 25 °C (Meylan and Howard, 1991) indicates that 1,4-butenediol is not expected to volatilize from water surfaces (Lyman et al., 1990). Hydrolysis is not expected to be an important fate process for 1,4-butenediol due to the lack of hydrolyzable functional groups (Lyman et al., 1990). No data were available in the scientific literature for the biodegradation of 1,4-butenediol in aquatic media under aerobic or anaerobic conditions. However, using a structure estimation

method (Boethling et al., 1994), aerobic biodegradation is expected to be rapid (days to weeks). According to a classification scheme (Franke et al., 1994), an estimated BCF of 0.14 (Lyman et al., 1990), obtained from the log Kow, suggests the potential for bioconcentration of 1,4-butenediol in aquatic organisms is low.

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), 1,4-butenediol, which has an extrapolated vapor pressure of 4.7×10^{-3} mm Hg at 25 °C (Grafje et al., 1985), is expected to exist solely as a gas in the ambient atmosphere. Gas-phase 1,4-butenediol is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 5-6 hours, depending upon the isomer (Meylan and Howard, 1993). The half-life for the reaction of 1,4-butenediol with ozone in the atmosphere is estimated to be 1-2 hours, depending upon the isomer (Meylan and Howard, 1993). 1,4-Butenediol is not expected to directly photolyze in the atmosphere due to the lack of absorption in the environmental UV spectrum greater than 290 nm (Lyman et al., 1990). Because 1,4-butenediol is miscible with water, physical removal from the atmosphere by wet deposition may occur.

C. Terrestrial Fate

An estimated Koc of 8.6 (Lyman, 1990), determined from a log Kow of -0.81 (Hansch et al., 1995), indicates that 1,4-butenediol is expected to have very high mobility in soil (Swann et al., 1983). Volatilization of 1,4-butenediol from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an estimated Henry's Law constant of 1.54×10^{-10} atm m³/mole (Meylan and Howard, 1991). In addition, an extrapolated vapor pressure of 4.7×10^{-3} mm Hg (Grafje et al., 1985) indicates that 1,4-butenediol is not expected to volatilize from dry soil surfaces. No data were available in the scientific literature for the biodegradation of 1,4-butenediol in soil under aerobic or anaerobic conditions. However, using a structure estimation method (Boethling et al., 1994), aerobic biodegradation is expected to be rapid (days to weeks).

D. Summary

1,4-Butenediol exists as a mixture of the cis and trans isomers that are expected to behave similarly in the environment. If released to air, an extrapolated vapor pressure of 4.7×10^{-3} mm Hg at 25 °C indicates 1,4-butenediol should exist solely as a gas in the ambient atmosphere. Gas-phase 1,4-butenediol will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 5-6 hours, depending upon the isomer. The gas phase reactions of 1,4-butenediol with photochemically produced ozone corresponds to a half-life of 1-2 hours. Physical removal of gas-phase 1,4-butenediol from the atmosphere may also occur via wet deposition processes based on the miscibility of this compound with water. If released to soil, 1,4-butenediol is expected to have very high mobility and is not expected to adsorb to soil surfaces. Volatilization from water and moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.54×10^{-10} atm m³/mole. In addition, volatilization from dry soil surfaces is not expected to occur based upon the vapor pressure of 1,4-butenediol. Biodegradation data were not available from the scientific literature; however, a computer model estimates that aerobic biodegradation in both soil and water may occur within days to weeks. In water, 1,4-butenediol is not expected to bioconcentrate in fish and aquatic organisms based on its estimated BCF of 0.14.

CHEMICAL SUMMARY FOR ACETIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of acetic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF ACETIC ACID

Characteristic/Property	Data	Reference
CAS No.	64-19-7	Howard and Neal (1992)
Common Synonyms	ethanoic acid; vinegar acid	Howard and Neal (1992)
Molecular Formula	C ₂ H ₄ O ₂	Budavari et al. (1996)
Chemical Structure	CH ₃ COOH	Budavari et al. (1996)
Physical State	clear liquid	Budavari et al. (1996)
Molecular Weight	60.05	Budavari et al. (1996)
Melting Point	16.7 °C	Budavari et al. (1996)
Boiling Point	118 °C	Budavari et al. (1996)
Water Solubility	1x10 ³ g/l, 25 °C	U.S. EPA (1981)
Density	d ^{25/25} , 1.049	Budavari et al. (1996)
Vapor Density (air = 1)	no data	
Koc	6.5-228	Sansone et al. (1987)
Log Kow	-0.17	Hansch et al. (1995)
Vapor Pressure	15.7 mm Hg @ 25 °C	Daubert and Danner (1985)
Reactivity	corrosive, particularly when dilute	Weiss (1986)
Flammability	flammable	Budavari et al. (1996)
Flash Point	103 °F (39 °C), closed cup	Budavari et al. (1996)
Dissociation Constant	pKa = 4.76	Serjeant and Dempsey (1979)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	1.00x10 ⁻⁹ atm m ³ /mole @ 25 °C	Gaffney et al. (1987)
Fish Bioconcentration Factor	<1 (calculated)	Lyman et al. (1990)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

The dominant environmental fate process for acetic acid in water is expected to be biodegradation. A large number of biological screening studies have determined that acetic acid biodegrades readily under both aerobic (Zahn and Wellens, 1980; Dore et al., 1975; Price et al., 1974; Placak and Ruchhoft, 1947 as cited in HSDB, 1998) and anaerobic (Kameya et al., 1995; Mawson et al., 1991; Swindoll et al., 1988 as cited in HSDB, 1998) conditions. Two aqueous adsorption studies found that acetic acid exists primarily in the water column and not in sediment (Hemphill and Swanson, 1964; Gordon and Millero, 1985 as cited in HSDB, 1998). In general, organic ions are not expected to volatilize from water to adsorb to particulate matter in water to the degree that would be predicted for

their neutral counterparts. Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990 as cited in HSDB, 1998) based on a Henry's Law constant of 1×10^{-9} atm-m³/mole at pH 7 (Gaffney et al., 1987 as cited in HSDB, 1998). According to a classification scheme (Franke et al., 1994 as cited in HSDB, 1998), an estimated BCF of <1 (Lyman, 1990 as cited in HSDB, 1998), calculated from a log K_{ow} of -0.17 (Hansch et al., 1995 as cited in HSDB, 1998), suggests that the potential for bioconcentration in aquatic organisms is low.

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988 as cited in HSDB, 1998), acetic acid, which has a vapor pressure of 15.7 mm Hg at 25 °C (Daubert and Danner, 1989 as cited in HSDB, 1998), should exist solely as a gas in the ambient atmosphere. This is consistent with a study in which over 91% of the total measured acetic acid in an air sample was found to be in the gas phase (Khawaja, 1995 as cited in HSDB, 1998). Acetic acid has been identified as one of the major sources of free acidity in precipitation from remote regions of the world (Keene and Galloway, 1984 as cited in HSDB, 1998), indicating that physical removal by wet deposition is an important fate process (Hartmann et al., 1989 as cited in HSDB, 1998). Another important removal process of acetic acid from the atmosphere is reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 22 days (Atkinson, 1989 as cited in HSDB, 1998). Acetic acid has also been detected adsorbed to atmospheric particulate material as the acetate (Gregory et al., 1986; Khawaja, 1995 as cited in HSDB, 1998); the small amount of acetic acid associated with particulate material may be physically removed by wet and dry deposition (Grosjean, 1992).

C. Terrestrial Fate

The major environmental fate process for acetic acid in soil is expected to be biodegradation. A large number of biological screening studies have determined that acetic acid biodegrades readily under both aerobic (Zahn and Wellens, 1980; Dore et al., 1975; Price et al., 1974; Placak and Ruchhoft, 1947 as cited in HSDB, 1998) and anaerobic (Kameya et al., 1995; Mawson et al., 1991; Swindoll et al., 1988 as cited in HSDB, 1998) conditions. Based on a classification scheme (Swann et al., 1983 as cited in HSDB, 1998), K_{oc} values of 6.5 to 228 (Sansone et al., 1987 as cited in HSDB, 1998) indicate that acetic acid is expected to have moderate to very high mobility in soil. This is consistent with a study in which no sorption was reported for three different soils/sediments (Von Oepen et al., 1991 as cited in HSDB, 1998). Volatilization of acetic acid from moist soil surfaces is not expected to be important (Lyman et al., 1990, as cited in HSDB, 1998) given a Henry's Law constant of 1×10^{-9} atm-m³/mole (Gaffney et al., 1987 as cited in HSDB, 1998) and because acetic acid will exist predominantly as the acetate at environmental pH's. However, the potential for volatilization of acetic acid from dry soil surfaces may exist based on its vapor pressure of 15.7 mm Hg (Daubert and Danner, 1989 as cited in HSDB, 1998). Volatilization will be attenuated depending upon pH and the amount of acetic acid dissociated.

D. Summary

Acetic acid occurs throughout nature as a normal metabolite of both plants and animals. Consequently, acetic acid's fate in the environment will, in part, be dependent on its participation in natural cycles. With a pK_a of 4.76, acetic acid and its conjugate base will exist in environmental media in varying proportions that are pH dependent; under typical environmental conditions (pHs of 5 to 9), acetic acid will exist almost entirely in the ionized (dissociated) form. If released to air, a vapor pressure of 15.7 mm Hg at 25 °C indicates that acetic acid should exist solely as a gas in the ambient atmosphere. Gas-phase acetic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 22 days. Physical removal of vapor-phase acetic acid from the atmosphere may occur via wet deposition processes based on its miscibility with water. An estimated BCF of <1 suggests the potential for bioconcentration on aquatic organisms is low. Adsorption studies indicate that acetic acid is not expected to adsorb to suspended solids and sediments in water. If released to soil, acetic acid is expected to have very high to moderate mobility based upon measured K_{oc} values ranging from 6.5 to 228 and, therefore, it has the potential to leach to groundwater. If released to soil in high concentrations, such as those encountered in a spill, acetic acid may travel through soil and reach groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon a Henry's Law constant of 1×10^{-9} atm-m³/mole. Yet, volatilization from dry soil surfaces may occur based upon the vapor pressure of this compound. However, volatilization of acetic acid will be pH dependent; if acetic acid is

dissociated, very little (about 1%) will be available for volatilization. Biodegradation is expected to be rapid and may be the dominant fate process in both soil and water under non-spill conditions; a large number of biological screening studies have determined that acetic acid biodegrades readily under both aerobic and anaerobic conditions.

CHEMICAL SUMMARY FOR BRANCHED OCTYLPHENOL, ETHOXYLATED¹
(alkylphenol polyethoxyethanol)

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for branched octylphenol, ethoxylated.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of branched octylphenol, ethoxylated¹ are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF BRANCHED OCTYLPHENOL, ETHOXYLATED¹

Characteristic/Property	Data	Reference
CAS No.	9036-19-5, 9002-93-1	Howard and Neal (1992)
Common Synonyms	Triton X-100 ¹ , OPIOSP	Howard and Neal (1992)
Molecular Formula	C ₁₄ H ₂₂ O.(C ₂ H ₄ O) ₁₀₀	Howard and Neal (1992)
Chemical Structure	(C ₈ H ₁₇)C ₆ H ₄ O(C ₂ H ₄ O) ₁₀₀	Howard and Neal (1992)
Physical State	Clear viscous liquid	MSDS
Molecular Weight	polymer, >4000	Howard and Neal (1992)
Melting Point	7.2°C	MSDS
Boiling Point	271°C	MSDS
Water Solubility	Dispersible, >100 g/L	MSDS
Density	d ₂₅ ²⁵ , 1.07	MSDS
Vapor Density (air = 1)	>1	MSDS
Koc	No data	
Log Kow	No data	
Vapor Pressure	<0.001 torr	MSDS
Reactivity	No data	
Flammability	No data	
Flash Point	288°C	MSDS
Dissociation Constant	No data	
Molecular Diffusivity Constant	No data	
Air Diffusivity Constant	No data	
Henry's Law Constant	No data	
Fish Bioconcentration Constant	No data	
Odor Threshold	No data	

¹ The properties are given for TritonX100 (manufacturer Rohm and Haas).

CHEMICAL SUMMARY FOR AMMONIUM CHLORIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ammonium chloride are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF AMMONIUM CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	12125-02-9	CAS (1998)
Common Synonyms	Ammonium muriate	Budavari et al. (1996)
Molecular Formula	ClH ₄ N	Budavari et al. (1996)
Chemical Structure	NH ₄ Cl	Budavari et al. (1996)
Physical State	colorless cubic crystals	Lide (1995)
Molecular Weight	53.492	Lide (1995)
Melting Point	sublimes at 350°C	Lewis (1993)
Boiling Point	no data	
Water Solubility	approximately 300 g/L ¹	Estimated
Density	1.519 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be < 10	Estimated
Log Kow	no data; expected to be < 1	Estimated
Vapor Pressure	1.84X10 ⁻¹² mm Hg at 25°C (extrapolated)	Daubert and Danner (1992)
Reactivity	no data	
Flammability	not flammable	Weiss (1986)
Flash Point	not flammable	Weiss (1986)
Dissociation Constant	dissociates to NH ₄ ⁺ and Cl ⁻	Bodek et al. (1988)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be < 1x10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	odorless	Weiss (1986)

¹ Estimated from a reported solubility of 37 parts in 100 parts water at 20°C (Dean 1985).

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If ammonium chloride is released into water, it is expected to dissociate into ammonium (NH₄⁺) and chloride (Cl⁻) ions (Bodek et al., 1988). The counter ion associated with the NH₄⁺ will vary depending on the concentration and type of ions available and the pH in the receiving water. In addition, NH₄⁺ and NH₃ (ammonia) are in equilibrium in the environment and since the pK_a of the ammonium ion, NH₄⁺, is 9.26, most ammonia in water is present as the protonated form rather than as NH₃ (Manahan, 1991). Ammonia is, however, present in the equilibrium and will volatilize to the atmosphere (based upon its Henry's Law constant of 1.6X10⁻⁵ atm m³/mole [Betterton, 1992 as cited in PHYSPROP, 1998]); the rate of volatilization will increase with increasing pH and, to a lesser degree, temperature

(ATSDR, 1990). In the aquatic environment, ammonium can undergo sequential transformation by the nitrification and denitrification processes of the nitrogen cycle; within this process, ionic nitrogen compounds are formed (ATSDR, 1990). In addition, ammonium can be taken up by aquatic plants as a source of nutrition, and the uptake of ammonium by fish has also been documented (ATSDR, 1990). Adsorption of ammonium to sediment should increase with increasing organic content, increased metal content, and decreasing pH; however, ammonium can be produced in, and subsequently released from, sediment (ATSDR, 1990). The dissociation of ammonium chloride into its component ions indicates that ammonium chloride is not expected to bioconcentrate in aquatic organisms. Ammonium ions may be adsorbed by negatively charged surfaces of sediment in the water column, however ammonium ions are expected to be replaced by other cations present in natural waters (Evans, 1989). The chloride ion may complex with heavy metals, thereby increasing their solubility (Bodek et al., 1988). Adsorption of the chloride ion to suspended solids and sediment in the water column is not expected to be an important fate process.

B. Atmospheric Fate

If ammonium chloride is released to the atmosphere, this compound's low vapor pressure (Daubert and Danner, 1992) indicates it will exist as a particulate in the ambient atmosphere. Ammonium chloride is expected to undergo wet deposition (ATSDR, 1990) in rain, snow, or fog based upon its high water solubility (Dean, 1985). Dry deposition of ammonium chloride is expected to be an important fate process in the atmosphere (ATSDR, 1990). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). In addition, NH_4^+ and NH_3 (ammonia) are in equilibrium. The gas-phase reactions of ammonia with photochemically produced hydroxyl radicals has been reported to be $1.6 \times 10^{-13} \text{ cm}^3/\text{mole} \cdot \text{sec}$, with a calculated half-life of approximately 100 days; this process contributes approximately 10% to the removal of atmospheric ammonia (ATSDR, 1990).

C. Terrestrial Fate

If ammonium chloride is released to soil, it is expected to dissociate into its component ions in moist soils. As noted above, NH_4^+ and NH_3 (ammonia) are in equilibrium in the environment and since the pK_a of the ammonium ion, NH_4^+ , is 9.26, most ammonia in water is present as the protonated form rather than as NH_3 (Manahan, 1991). The low vapor pressure and Henry's Law constant expected for an ionic salt indicates that ammonium chloride will not volatilize from either dry or moist soil surfaces. Nonetheless, ammonia is present in the equilibrium and will volatilize to the atmosphere (based upon its Henry's Law constant of $1.6 \times 10^{-5} \text{ atm} \cdot \text{m}^3/\text{mole}$ [Betterton, 1992 as cited in PHYSPROP, 1998]); the rate of volatilization will increase with increasing pH and, to a lesser degree, temperature (ATSDR, 1990). The mobility of ammonium ions through soil may be attenuated by attraction to negatively charged surfaces of soil particles, however ammonium ions are expected to be replaced by other cations present in soil (Evans, 1989). In soil, ammonium will serve as a source of nutrient taken up by plants and other organisms and converted to organic-nitrogen compounds. Ammonium can be converted to nitrate by microbial populations through nitrification; the nitrate formed will either leach through soil or be taken up by plants and other organisms. It has been determined that minerals and dry soils can rapidly and effectively adsorb ammonia from air. Chloride is extremely mobile in soils (Bodek et al., 1988). The chloride ion may complex with heavy metals, thereby increasing their solubility (Bodek et al., 1988) and potential for leaching into groundwater.

D. Summary

If released into water, ammonium chloride is expected to dissociate into ammonium and chloride ions. The dissociation of ammonium chloride into its component ions indicates that ammonium chloride is not expected to bioconcentrate in aquatic organisms. Ammonium, however, will be used as a nutrient source by microorganisms and plants, and rapid uptake is anticipated. Ammonium is in equilibrium with ammonia, but the majority will be in the ammonium form under most environmental pHs. When present, ammonia's Henry's Law constant indicates that volatilization from water surfaces may occur. If released to soil, ammonium chloride is expected to dissociate into its component ions in moist soils and will be used as a nutrient by microorganisms and plants. The dissociation of ammonium chloride into its component ions in moist soils indicates that volatilization of ammonium from moist soil surfaces is not expected to occur. The mobility of ammonium ions in soil is expected to be attenuated by cation exchange processes. The low vapor pressure expected for an ionic salt indicates that ammonium chloride is not expected to volatilize from dry soil surfaces, however, when ammonia is present in equilibrium, volatilization may

occur. If released to the atmosphere, ammonium chloride's low vapor pressure indicates this compound will exist as a particulate. Wet and dry deposition will be the dominant fate processes in the atmosphere. The rate of dry deposition will depend on the prevailing wind patterns and particle size. Some atmospheric oxidation may occur.

CHEMICAL SUMMARY FOR AMMONIUM HYDROXIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ammonium hydroxide are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF AMMONIUM HYDROXIDE

Characteristic/Property	Data	Reference
CAS No.	1336-21-6	Lide (1995)
Common Synonyms	ammonia solution; aqua ammonia; ammonium hydrate	Lewis (1993)
Molecular Formula	H_3NO	PHYSPROP (1998)
Chemical Structure	NH_4OH	Lide (1995)
Physical State	colorless liquid	Lewis (1993)
Molecular Weight	35.05	Lide (1995)
Melting Point	no data	
Boiling Point	no data	
Water Solubility	soluble in water	Sax (1984)
Density	no data	
Vapor Density (air = 1)	no data	
Koc	no data; estimated to be < 10	Estimated
Log Kow	no data; estimated to be < 1	Estimated
Vapor Pressure	no data	
Reactivity	incompatible w/ HCl, HNO ₃ , Ag compounds	Sax (1984)
Flammability	not flammable	Weiss (1986)
Flash Point	no data; estimated to be > 350 °C	Estimated
Dissociation Constant	9.26 (water solution)	Manahan (1991)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data ¹	
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ In the environment, ammonium ion is expected to predominate in the ammonia-ammonium ion equilibrium; however, this equilibrium is highly dependent on both pH and temperature (ATSDR, 1990). Ammonia is expected to have a very high Henry's Law constant, while ammonium is expected to have a negligible Henry's Law constant (SRC, 1998).

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into the water column at low concentrations, ammonia or ammonium hydroxide will volatilize to the atmosphere; the rate of volatilization will increase with increasing pH and, to a lesser degree, temperature (ATSDR, 1990). Since the pKa of the ammonia is 9.26, most ammonia in most environmental waters is present as the protonated, NH_4^+ , form rather than as NH_3 (Manahan, 1991). In the aquatic environment, ammonia can undergo

sequential transformation by the nitrification and denitrification processes of the nitrogen cycle; within this process, ionic nitrogen compounds are formed (ATSDR, 1990). In addition, ammonia can be taken up by aquatic plants as a source of nutrition, and the uptake of ammonia by fish has also been documented (ATSDR, 1990). Adsorption of ammonia to sediment should increase with increasing organic content, increased metal content, and decreasing pH; however, ammonia can be produced in, and subsequently released from sediment (ATSDR, 1990). Large releases of the concentrated base into water, such as may result from a spill, will result in an increase of the pH (ATSDR, 1990).

B. Atmospheric Fate

If ammonia is released to the atmosphere, its vapor pressure indicates it will exist as a vapor in the ambient atmosphere. If ammonium hydroxide is released to the atmosphere, it is anticipated that the dominant form will be as a particulate, but during equilibrium between ammonium and ammonia, the ammonia will rapidly leave the particle as a vapor. The dominant fate process for the removal of ammonia from the atmosphere is the reaction with acid air pollutants to form ammonium compounds (e.g., ammonium sulfate, ammonium nitrate); these ammonium compounds can then be removed by wet or dry deposition (ATSDR, 1990). In addition, gas-phase reactions of ammonia with photochemically produced hydroxyl radicals has been reported to be 1.6×10^{-13} cm³/mol-sec, with a calculated half-life of approximately 100 days; this process contributes approximately 10% to the removal of atmospheric ammonia (ATSDR, 1990).

C. Terrestrial Fate

If ammonia or ammonium hydroxide is released to soil, it will serve as a source of nutrient taken up by plants and other organisms and converted to organic-nitrogen compounds. Ammonia can be converted to nitrate by microbial populations through nitrification; the nitrate formed will either leach through soil or be taken up by plants and other organisms. It has been determined that minerals and dry soils can rapidly and effectively adsorb ammonia from air. Specifically, ammonia may be either bound to soil or undergo volatilization to the atmosphere. (ATSDR, 1990)

D. Summary

Ammonia is a base, and as such, the environmental fate of ammonia is pH and temperature dependent. If released into water, ammonia and ammonium hydroxide will volatilize to the atmosphere, depending on the pH. At high pHs, where the equilibrium more favors ammonia, volatilization will become increasingly important. At low pHs, volatilization will be less important. Adsorption of ammonia to sediment and suspended organic material can be important under proper conditions (i.e., organic matter content, metal content, and pH). In addition, ammonia will be taken up by aquatic organisms and plants as a source of nutrition. The dominant fate of ammonia in water will be its participation in the nitrogen cycle. The predominant removal process of ammonia and ammonium hydroxide from the atmosphere is expected to be wet and dry deposition. To a lesser extent, reactions with photochemically-produced hydroxyl radicals will occur. If released to soil, ammonia is expected to be taken up by plants and other organisms and converted to organic-nitrogen compounds. These compounds will either be taken up by plants or other organisms or leach through the soil. Volatilization of ammonia from soil surfaces is expected to occur.

CHEMICAL SUMMARY FOR SODIUM CITRATE (citric acid)

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of sodium citrate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM CITRATE

Characteristic/Property	Data	Reference
CAS No.	68-04-2	
Common Synonyms	trisodium citrate; sodium citrate anhydrous; 2-hydroxy-1,2,3-propanetricarboxylic acid, trisodium salt	Lockheed Martin 1991
Molecular Formula	$C_6H_5Na_3O_7$	Budavari et al. 1989
Chemical Structure	$CH_2(COONa)C(OH)(COONa)CH_2COONa$	Osol 1980
Physical State	dihydrate, white crystals, granules, or powder; pentahydrate, relatively large, colorless crystals or white granules	Budavari et al. 1989
Molecular Weight	258.07	Budavari et al. 1989
Melting Point	150 °C (-2 H ₂ O)	Fisher Scientific 1985
Boiling Point	decomposed at red heat	Lewis 1993
Water Solubility	72 g/100 mL at 25 °C (dihydrate)	Weast 1983-1984
Density	1.9	Fisher Scientific 1985
Vapor Density (air = 1)	no data	
K _{OC}	no data	
Log K _{OW}	no data	
Vapor Pressure	no data	
Reactivity	0 (nonreactive, NFPA classification); aqueous solution slightly acid to litmus	Lockheed Martin 1991 Osol, 1980
Flammability	1 (slightly combustible, NFPA classification);	Lockheed Martin 1991
Flash Point	no data	
Dissociation Constant	no data	
Henry's Law Constant	no data	
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	no data; odorless	Lewis 1993
Conversion Factors	no data	

II. ENVIRONMENTAL FATE

A. Environmental Release

Sodium citrate is a solid with a cool, saline taste that is soluble in water (Fisher Scientific 1985). It is used in soft drinks, frozen desserts, meat products, cheeses, and as a nutrient for cultured buttermilk; in photography; in detergents; as a sequestrant and buffer; as an anticoagulant for blood withdrawn from the body; and in the removal of sulfur dioxide from smelter waste gases (Lewis 1993). Medicinally, sodium citrate is used as expectorant and

systemic alkalizer. Sodium citrate is a chelating agent and has been used to facilitate elimination of lead from the body (Osol 1980).

No data were found on the environmental releases of sodium citrate. The chemical is not listed on U.S. EPA's Toxics Release Inventory, requiring certain U.S. industries to report on chemical releases to the environment (TRI93 1995). The chemical could potentially enter the environment when used for the removal of sulfur dioxide from smelter waste gases.

B. Transport

No data were found on the environmental transport of sodium citrate in the secondary sources searched. Its water solubility suggests that the sodium citrate would remain in the water phase.

C. Transformation/Persistence

No data were found on the transformation/persistence of potassium bisulfate in the secondary sources searched.

CHEMICAL SUMMARY FOR CUPRIC SULFATE (copper ion)

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of cupric sulfate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF CUPRIC SULFATE

Characteristic/Property	Data	Reference
CAS No.	7758-99-8	Lide (1995)
Common Synonyms	cupric sulfate pentahydrate; blue Vitriol	Budavari et al. (1996)
Molecular Formula	$\text{CuO}_4\text{S}\cdot 5\text{H}_2\text{O}$	ATSDR (1990)
Chemical Structure	$\text{CuSO}_4\cdot 5\text{H}_2\text{O}$	Lide (1995)
Physical State	large, blue, triclinic crystals; blue powder	Budavari et al. (1996)
Molecular Weight	249.68	Lide (1995)
Melting Point	decomposes @ 110°C	Lide (1995)
Boiling Point	decomposes to CuO @ 650°C	ATSDR (1990)
Water Solubility	316 g/L @ 0°C	Weast et al. (1985)
Density	2.286 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data	
Log Kow	no data	
Vapor Pressure	no data	
Reactivity	reacts with Mg to produce Cu_2O , MgSO_4 , and H_2	U.S. Air Force (1990)
Reactivity	reacts with NH_4Cl producing $(\text{NH}_4)_2\text{SO}_4$ and CuCl_2 ; reacts with alkali (R)OH to produce $\text{Cu}(\text{OH})_2$ and RSO_4 ; reacts with excess aq. NH_3 producing $\text{Cu}(\text{NH}_3)_2^{2+} + \text{OH}^-$; decomposition products include SO_2 .	HSDB (1998)
Flammability	non-flammable	HSDB (1998)
Flash Point	non-flammable	HSDB (1998)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data	
Fish Bioconcentration Constant	10-100 for copper; 30,000 for copper in oysters	ATSDR (1990)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Copper (Cu) commonly exists in three valence states, Cu^0 (metal), Cu^+ (cuprous), and Cu^{2+} (cupric). It can also be oxidized to a Cu^{3+} state, but Cu^{3+} ions are rapidly reduced to Cu^{2+} in the environment (ATSDR, 1990). Copper in solution is present almost exclusively as the Cu^{2+} valence state (U.S. EPA, 1987). Copper in the Cu^{2+} valence state

forms compounds and complexes with a variety of organic and inorganic ligands binding to -NH_2 , -SH , and, to a lesser extent, -OH groups (ATSDR, 1990). The predominant form of copper in aqueous solution is dependent on the pH of the solution. Below pH 6, the cupric ion (Cu^{2+}) predominates; copper complexes with carbonate usually predominate above pH 6 (U.S. EPA, 1987; ATSDR, 1990). The association of copper with organic or inorganic ligands also depends on the pH and on the CaCO_3 alkalinity. Most of the copper entering surface water is in the form of particulate matter, which settles out, precipitates, or adsorbs to organic matter, hydrous iron and manganese oxides, and clay; however, the predominating form can change with the amount of rain, pH, content of runoff, and the availability of ligands (ATSDR, 1990). The processes of complexation, adsorption and precipitation limit the concentration of copper (Cu^{2+}) to very low values in most natural waters (ATSDR, 1990). Calculations of the bioconcentration factor in fish for copper have ranged from 10 to 100; however, the majority of copper measurements in fish tissues under environmental conditions have indicated little, if any, bioconcentration. Filter feeding shellfish, especially oysters, however, were found to significantly concentrate copper with bioconcentration factors as high as 30,000 (ATSDR, 1990).

B. Atmospheric Fate

Most of the copper in the air is in the form of particulate matter (dust) or is adsorbed to particulate matter. Larger particles ($>5\ \mu\text{m}$) are removed by gravitational settling, smaller particles are removed by other forms of dry and wet deposition (ATSDR, 1990). Atmospheric copper resulting from combustion is associated with sub-micron particles that can remain in the troposphere for an estimated 7-30 days and may be carried long distances (ATSDR, 1990).

C. Terrestrial Fate

Most of the copper deposited in the soil is strongly adsorbed primarily to organic matter, carbonate minerals, clay minerals, and hydrous iron and manganese oxides. Movement through the soil is dependent on the presence of these substances, the pH, and other physical and chemical parameters. The greatest potential for leaching is seen in sandy soils with low pH (ATSDR, 1990). Laboratory experiments using controlled models and field experiments utilizing core samples have shown that very little copper moves through the soil. Core samples showed that some movement occurred as far as the 22.5-25 cm layer of soil, but little, if any, moved below this zone. The evidence indicates that hazardous amounts of copper should not leach into groundwater from sludge, even from sandy soils (ATSDR, 1990).

D. Summary

Copper (Cu) commonly exists in three valence states, Cu^0 (metal), Cu^+ (cuprous), and Cu^{2+} (cupric). It can also be oxidized to a Cu^{3+} state, but there are no important industrial Cu^{3+} chemicals, and Cu^{3+} ions are rapidly reduced to Cu^{2+} in the environment. If released to water, copper in solution will be present almost exclusively as the Cu^{2+} valence state. The predominant form of copper in aqueous solution is dependent on the pH of the solution. Most of the copper entering surface water is in the form of particulate matter; however, the predominating form can change with the amount of rain, pH, content of runoff, and the availability of ligands. Copper in the Cu^{2+} valence state will form compounds and complexes with a variety of organic and inorganic ligands. Calculations of the bioconcentration factor in fish for copper have ranged from 10 to 100; however, the majority of copper measurements in fish tissues under environmental conditions have indicated little, if any, bioconcentration. If released to soil, the majority of copper deposited in the soil is strongly adsorbed. Movement through the soil is dependent on the presence of organic matter, carbonate minerals, clay minerals, hydrous iron and manganese oxides, the pH, and other physical and chemical parameters. The greatest potential for leaching is seen in sandy soils with low pH. If released into the atmosphere, copper is expected to exist as a dust particulate or adsorb to particulate matter. Studies have shown that copper can remain in the atmosphere up to 30 days and be carried long distances.

CHEMICAL SUMMARY FOR CUPRIC ACETATE (copper sulfate pentahydrate)

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of cupric acetate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF COPPER ACETATE

Characteristic/Property	Data	Reference
CAS No.	6046-93-1	Lide (1995)
Common Synonyms	copper (II) acetate monohydrate	Lide (1995)
Molecular Formula	$(\text{CH}_3\text{CO}_2)_2\text{Cu}\cdot\text{H}_2\text{O}$	Aldrich (1996)
Chemical Structure	$\text{Cu}(\text{C}_2\text{H}_3\text{O}_2)_2\cdot\text{H}_2\text{O}$	Lide (1995)
Physical State	dark, green monoclinic crystals	Budavari et al. (1996)
Physical State	greenish-blue, fine powder	Lewis (1993)
Molecular Weight	199.65	Lide (1995)
Melting Point	115 °C	Lide (1995)
Boiling Point	decomposes at 240 °C	Lide (1995)
Water Solubility	72 g/L cold water; 200 g/L hot water	Weast et al. (1985)
Density	1.88 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data	
Log Kow	no data	
Vapor Pressure	no data	
Reactivity	stable	Weiss (1986)
Flammability	not flammable	Weiss (1986)
Flash Point	not flammable	Weiss (1986)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data	
Fish Bioconcentration Constant	10-100 for copper; 30,000 for copper in oysters	ATSDR (1990)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Copper (Cu) commonly exists in three valence states, Cu⁰ (metal), Cu⁺ (cuprous), and Cu²⁺ (cupric). It can also be oxidized to a Cu³⁺ state, but Cu³⁺ ions are rapidly reduced to Cu²⁺ in the environment (ATSDR, 1990). Copper in solution is present almost exclusively as the Cu²⁺ valence state (U.S. EPA, 1987). Copper in the Cu²⁺ valence state forms compounds and complexes with a variety of organic and inorganic ligands binding to -NH₂, -SH, and, to a lesser extent, -OH groups (ATSDR, 1990). The predominant form of copper in aqueous solution is dependent on the pH of the solution. Below pH 6, the cupric ion (Cu²⁺) predominates; copper complexes with carbonate usually

predominate above pH 6 (U.S. EPA, 1987; ATSDR, 1990). The association of copper with organic or inorganic ligands also depends on the pH and on the CaCO_3 alkalinity. Most of the copper entering surface water is in the form of particulate matter, which settles out, precipitates, or adsorbs to organic matter, hydrous iron and manganese oxides, and clay; however, the predominating form can change with the amount of rain, pH, content of runoff, and the availability of ligands (ATSDR, 1990). The processes of complexation, adsorption and precipitation limit the concentration of copper (Cu^{2+}) to very low values in most natural waters (ATSDR, 1990). Calculations of the bioconcentration factor in fish for copper have ranged from 10 to 100; however, the majority of copper measurements in fish tissues under environmental conditions have indicated little, if any, bioconcentration. Filter feeding shellfish, especially oysters, however, were found to significantly concentrate copper with bioconcentration factors as high as 30,000 (ATSDR, 1990).

B. Atmospheric Fate

Most of the copper in the air is in the form of particulate matter (dust) or is adsorbed to particulate matter. Larger particles ($>5\ \mu\text{m}$) are removed by gravitational settling, smaller particles are removed by other forms of dry and wet deposition (ATSDR, 1990). Atmospheric copper resulting from combustion is associated with sub-micron particles that can remain in the troposphere for an estimated 7-30 days and may be carried long distances (ATSDR, 1990).

C. Terrestrial Fate

Most of the copper deposited in the soil is strongly adsorbed primarily to organic matter, carbonate minerals, clay minerals, and hydrous iron and manganese oxides. Movement through the soil is dependent on the presence of these substances, the pH, and other physical and chemical parameters. The greatest potential for leaching is seen in sandy soils with low pH (ATSDR, 1990). Laboratory experiments using controlled models and field experiments utilizing core samples have shown that very little copper moves through the soil. Core samples showed that some movement occurred as far as the 22.5-25 cm layer of soil, but little, if any, moved below this zone. The evidence indicates that hazardous amounts of copper should not leach into groundwater from sludge, even from sandy soils (ATSDR, 1990).

D. Summary

Copper (Cu) commonly exists in three valence states, Cu^0 (metal), Cu^+ (cuprous), and Cu^{2+} (cupric). It can also be oxidized to a Cu^{3+} state, but there are no important industrial Cu^{3+} chemicals, and Cu^{3+} ions are rapidly reduced to Cu^{2+} in the environment. If released to water, copper in solution will be present almost exclusively as the Cu^{2+} valence state. The predominant form of copper in aqueous solution is dependent on the pH of the solution. Most of the copper entering surface water is in the form of particulate matter; however, the predominating form can change with the amount of rain, pH, content of runoff, and the availability of ligands. Copper in the Cu^{2+} valence state will form compounds and complexes with a variety of organic and inorganic ligands. Calculations of the bioconcentration factor in fish for copper have ranged from 10 to 100; however, the majority of copper measurements in fish tissues under environmental conditions have indicated little, if any, bioconcentration. If released to soil, the majority of copper deposited in the soil is strongly adsorbed. Movement through the soil is dependent on the presence of organic matter, carbonate minerals, clay minerals, hydrous iron and manganese oxides, the pH, and other physical and chemical parameters. The greatest potential for leaching is seen in sandy soils with low pH. If released into the atmosphere, copper is expected to exist as a dust particulate or adsorb to particulate matter. Studies have shown that copper can remain in the atmosphere up to 30 days and be carried long distances.

CHEMICAL SUMMARY FOR ETHYLENEDIAMINE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ethylene diamine are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF ETHYLENE DIAMINE

Characteristic/Property	Data	Reference
CAS No.	107-15-3	Howard and Neal (1992)
Common Synonyms	1,2-diamineethane; 1,2-ethanediamine	Budavari et al. (1996)
Molecular Formula	C ₂ H ₈ N ₂	Budavari et al. (1996)
Chemical Structure	H ₂ NCH ₂ CH ₂ NH ₂	Budavari et al. (1996)
Physical State	colorless, clear, thick, liquid	Budavari et al. (1996)
Molecular Weight	60.10	Budavari et al. (1996)
Melting Point	8.5 °C	Budavari et al. (1996)
Boiling Point	116-117 °C	Budavari et al. (1996)
Water Solubility	1x10 ³ g/l @ 25 °C	Riddick et al. (1986)
Density	d ^{25/4} , 0.898	Budavari et al. (1996)
Vapor Density (air = 1)	no data	
Koc	2 (calculated)	Lyman et al. (1990)
Log Kow	-2.04	Hansch et al. (1995)
Vapor Pressure	12.0 mm Hg @ 25 °C	Boublik et al. (1984)
Reactivity	volatile w/ steam; absorbs CO ₂ from air	Budavari et al. (1996)
Flammability	flammable	Aldrich (1997)
Flash Point	110 °F (43 °C), closed cup	Budavari et al. (1996)
Dissociation Constant	pKa ₁ = 9.92; pKa ₂ = 6.86	Perrin (1972)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	1.73x10 ⁻⁹ atm m ³ /mole @ 25 °C	Hine and Mookerjee (1975)
Fish Bioconcentration Factor	0.02 (calculated)	Lyman et al. (1990)
Odor Threshold	100% recognizable @ 11.2 ppm	Verschueren (1996)

II. ENVIRONMENTAL FATE

A Aquatic Fate

The dominant environmental fate process for ethylenediamine in surface water is expected to be biodegradation. A number of biological screening studies have determined that ethylenediamine biodegrades readily under aerobic conditions (Price et al., 1974; Takemoto et al., 1981; Pitter, 1976 ; Mills and Stack, 1955, as cited in HSDB, 1998). No data were available for the biodegradation of ethylenediamine under anaerobic conditions. An estimated Koc value of 2, determined from an experimental log Kow of -2.04 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990), indicates that ethylenediamine is not expected to adsorb to suspended solids and sediment in water. In general, organic ions are not expected to volatilize from water or adsorb to particulate matter in water to the degree that would be predicted for their neutral counterparts. Based on an estimated BCF of 0.02

(Lyman et al., 1990) calculated from the log Kow, a classification scheme (Franke et al., 1994) suggests the potential for bioconcentration in aquatic organisms is low. Ethylenediamine is not expected to volatilize from water surfaces (Lyman et al., 1990) based upon an experimental Henry's Law constant of 1.73×10^{-9} atm-m³/mole (Hine and Mookerjee, 1975). However, volatilization of ethylenediamine will be pH dependent and attenuated if it is protonated; very little, about 1%, will be available for volatilization. Hydrolysis of ethylenediamine is not expected to occur due to the lack of hydrolyzable functional groups (Lyman et al., 1990).

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), ethylenediamine, which has a vapor pressure of 12 mm Hg at 25 °C (Boublik et al., 1984), should exist solely as a gas in the ambient atmosphere. Gas-phase ethylenediamine is degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 6 hours (Meylan and Howard, 1993). Due to its miscibility with water, ethylenediamine may also be removed physically from the atmosphere by wet deposition. Ethylenediamine is not expected to directly photolyze in the atmosphere due to the lack of absorption in the environmental UV spectrum (>290 nm) (Lyman et al., 1990).

C. Terrestrial Fate

The major environmental fate process for ethylenediamine in aerobic soils is expected to be biodegradation. A number of biological screening studies have determined that ethylenediamine biodegrades readily under aerobic conditions (Price et al., 1974; Takemoto et al., 1981; Pitter, 1976; Mills and Stack, 1955, as cited in HSDB, 1998). No data on the biodegradation of ethylenediamine under anaerobic conditions were located in the available literature. An estimated Koc value of 2 (Lyman et al., 1990), determined from an experimental log Kow of -2.04 (Hansch et al., 1995), indicates that ethylenediamine is expected to have very high mobility in soil (Swann et al., 1983). Volatilization of ethylenediamine from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an experimental Henry's Law constant of 1.73×10^{-9} atm-m³/mole (Hine and Mookerjee, 1975), although it may volatilize from dry soil surfaces based upon a vapor pressure of 12 mm Hg (Boublik et al., 1984). However, at environmental pH's of 5-7, ethylenediamine will most likely be a salt and volatilization will be attenuated.

D. Summary

The dominant removal mechanisms of ethylenediamine from the environment are expected to be biodegradation on the earth's surface and reaction with photochemically-produced hydroxyl radicals in the atmosphere. In both soil and water, biodegradation is expected to be rapid; a large number of biological screening studies have determined that ethylenediamine biodegrades readily under aerobic conditions. If released to air, a vapor pressure of 12 mm Hg indicates ethylenediamine should exist solely as a gas in the ambient atmosphere. Gas-phase ethylenediamine will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 6 hours. Physical removal of gas-phase ethylenediamine from the atmosphere may also occur via wet deposition processes based on the miscibility of this compound with water. With a pK_{a1} of 9.92, ethylenediamine and its conjugate acid will exist in environmental media in varying proportions that are pH dependent. If released to soil, ethylenediamine may display very high mobility based upon an estimated Koc of 2. If released to soil in high concentrations, such as those encountered in a spill, ethylenediamine may travel through soil and reach groundwater. Volatilization of ethylenediamine from water and moist soil surfaces is not expected to be an important fate process based upon a Henry's Law constant of 1.73×10^{-9} atm-m³/mole, although its vapor pressure indicates that volatilization from dry soil surfaces may occur. However, at environmental pH's of 5-7, ethylenediamine will most likely be a salt and volatilization will be attenuated. In water, ethylenediamine is not expected to bioconcentrate in fish and aquatic organisms based on an estimated BCF of 0.02.

CHEMICAL SUMMARY FOR ETHYLENE GLYCOL

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ethylene glycol are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF ETHYLENE GLYCOL

Characteristic/Property	Data	Reference
CAS No.	107-21-1	Budavari et al. (1996)
Common Synonyms	1,2-ethanediol	Budavari et al. (1996)
Molecular Formula	C ₂ H ₆ O ₂	Budavari et al. (1996)
Chemical Structure	HOCH ₂ CH ₂ OH	Budavari et al. (1996)
Physical State	slightly viscous liquid	Budavari et al. (1996)
Molecular Weight	62.07	Budavari et al. (1996)
Melting Point	-13 °C	Budavari et al. (1996)
Boiling Point	197.6 °C	Budavari et al. (1996)
Water Solubility	miscible (1,000 g/l)	Riddick et al (1986)
Density	1.11 g/cm ³	Budavari et al. (1996)
Vapor Density (air = 1)	2.1	Verschueren (1996)
Koc	4 (estimated)	SRC (1998)
Log Kow	-1.36	Hansch et al. (1995), as cited in HSDB (1998)
Vapor Pressure	0.092 mm Hg	Daubert and Danner (1989)
Reactivity	no data	no data
Flammability	combustible	Lewis (1993)
Flash Point	240 °F (115 °C)	Budavari et al. (1996)
Dissociation Constant	15.1	Howard and Meylan (1997)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	6.0x10 ⁻⁸ atm m ³ /mol	Howard and Meylan (1997)
Fish Bioconcentration Constant	10	HSDB (1998)
Odor Threshold	25 ppm	ECDIN (1998)

II. ENVIRONMENTAL FATE

A. Aquatic Fate

The dominant environmental fate process for ethylene glycol in water is expected to be biodegradation. A large number of biological screening studies have determined that ethylene glycol biodegrades readily under both aerobic and anaerobic conditions (Bridie et al. 1979; Pitter 1976; and Price et al. 1974, as cited in HSDB, 1998). Aerobic degradation is essentially complete in <1-4 days, although 100% theoretical biological oxygen demand may not be realized for several weeks (Bridie et al., 1979; Pitter 1976; and Price et al., 1974, as cited in HSDB, 1998). Ethylene glycol is not expected to adsorb to suspended solids and sediments in water based upon an estimated Koc of 4 (Swann et al., 1983, as cited in HSDB, 1998), determined from a log Kow of -1.36 (Hansch et al., 1995, as cited in

HSDB, 1998) and a regression-derived equation (Lyman et al., 1990, as cited in HSDB, 1998). Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990, as cited in HSDB, 1998) based on a Henry's Law constant of 6.0×10^{-8} atm-m³/mole (Butler and Ramchandani 1935, as cited in Howard and Meylan 1997). Ethylene glycol is expected to be stable to hydrolysis in the pH range of 5-9 typically encountered in the environment (Lyman et al., 1990, as cited in HSDB, 1998). According to a classification scheme (Franke et al., 1994), a BCF of 10 in golden ide fish (Freitag et al., 1985, as cited in HSDB, 1998) suggests that the potential for bioconcentration in aquatic organisms is low.

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman 1989, as cited in HSDB, 1998), ethylene glycol, which has a vapor pressure of 0.092 mm Hg at 25 °C (Daubert and Danner 1989), should exist solely as a gas in the ambient atmosphere. Nonetheless, ethylene glycol has been detected adsorbed onto atmospheric particulate material (Abdelghani et al., 1990, as cited in HSDB, 1998); the small amount of ethylene glycol deposited onto particulate material may be physically removed by wet and dry deposition. The predominant removal process of ethylene glycol from the atmosphere is reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 50 hours (Atkinson 1989, as cited in HSDB, 1998). Ethylene glycol may undergo some degradation by direct photolysis; 12.1% of applied ethylene glycol was degraded after 17 hours following irradiation by light > 290 nm (Freitag et al., 1985, as cited in HSDB, 1998).

C. Terrestrial Fate

The major environmental fate process for ethylene glycol in soil is expected to be biodegradation. A large number of biological screening studies have determined that ethylene glycol biodegrades readily under both aerobic and anaerobic conditions; complete biodegradation was shown in one soil within 2 days and 97% biodegradation in 12 days was reported for a second soil (McGahey and Bower 1992, as cited in HSDB, 1998). Based on a classification scheme (Swann et al., 1983, as cited in HSDB, 1998), an estimated Koc of 4, determined from a log Kow of -1.36 (Hansch et al., 1995, as cited in HSDB, 1998) and a regression-derived equation (Lyman, 1990 et al., as cited in HSDB, 1998), indicates that ethylene glycol is expected to have very high mobility in soil. Percent adsorption to 4 soils (2 clay and 2 sandy clay soils) ranged from 0-0.5% (Abdelghani et al 1990, as cited in HSDB, 1998). Volatilization of ethylene glycol from moist soil surfaces is not expected to be important (Lyman et al., 1990, as cited in HSDB, 1998) given a Henry's Law constant of 6.0×10^{-8} atm-m³/mole (Butler and Ramchandani 1935, as cited in Howard and Meylan 1997). Ethylene glycol may volatilize from dry soil given its vapor pressure of 0.092 mm Hg (Daubert and Danner, 1989); this may be attenuated by hydrogen bonding to soil materials (SRC, 1998).

D. Summary

If released to air, a vapor pressure of 0.092 mm Hg at 25 °C indicates that ethylene glycol should exist solely as a gas in the ambient atmosphere; however, experimental results show that at least some ethylene glycol is associated with atmospheric particulates. Gas-phase ethylene glycol will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 50 hours. Adsorption studies indicate that ethylene glycol is not expected to adsorb to suspended solids and sediments in water. A BCF of 10 in golden ide fish suggests the potential for bioconcentration in aquatic organisms is low. If released to soil, ethylene glycol is expected to have very high mobility based upon an estimated Koc of 4, and, therefore, it has the potential to leach to groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon a Henry's Law constant of 6.0×10^{-8} atm-m³/mole. Volatilization from dry soil surfaces may occur based upon the vapor pressure of this compound, although this may be attenuated by hydrogen bonding to soil materials. Biodegradation is expected to be rapid and may be the dominant fate process in both soil and water under non-spill conditions; a large number of biological screening studies have determined that ethylene glycol biodegrades readily under both aerobic and anaerobic conditions.

CHEMICAL SUMMARY FOR ETHYLENE GLYCOL MONOBUTYL ETHER

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for ethylene glycol monobutyl ether.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of ethylene glycol monobutyl ether are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF ETHYLENE GLYCOL MONOBUTYL ETHER

Characteristic/Property	Data	Reference
CAS No.	111-76-2	Howard and Neal (1992)
Common Synonyms	BUCS, butoxyethanol, Dowanol EB	Howard and Neal (1992)
Molecular Formula	C ₆ H ₁₄ O ₂	Howard and Neal (1992)
Chemical Structure	CH ₃ (CH ₂) ₃ OCH ₂ CH ₂ OH	Howard and Neal (1992)
Physical State	Clear, colorless liquid	HSDB (1998)
Molecular Weight	118.18	Howard and Neal (1992)
Melting Point	-70°C	Budavari et al. (1996)
Boiling Point	171°C, 743 mm Hg	Budavari et al. (1996)
Water Solubility	>1000 g/L, 25°C	HSDB (1998)
Density	d ^{20/20} , 0.9012	HSDB (1998)
Vapor Density (air = 1)	4.07	HSDB (1998)
Koc	1	EPI
Log Kow	0.83	Howard and Meylan (1997)
Vapor Pressure	0.88 mm Hg @ 25°C	Howard and Meylan (1997)
Reactivity	Inert	Sax and Lewis (1987)
Flammability	Combustible	Sax and Lewis (1987)
Flash Point	60°C	HSDB (1998)
Dissociation Constant	No data	
Molecular Diffusivity Constant	No data	
Air Diffusivity Constant	No data	
Henry's Law Constant	2.08x10 ⁻⁸ atm m ³ /mol	Howard and Meylan (1997)
Fish Bioconcentration Constant	No data	
Odor Threshold	No data	

CHEMICAL SUMMARY FOR FLUOROBORIC ACID (fluoride)

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper and tin-palladium processes. This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. Very little information on the environmental fate and toxicity of fluoroboric acid or fluoroborates was found in the available secondary sources. Supplemental information is provided for fluoride which may be a degradation product and for sodium bifluoride.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of fluoroboric acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF FLUOROBORIC ACID

Characteristic/Property	Data	Reference
CAS No.	16872-11-0	HSDB (1995)
Common Synonyms	hydrogen tetrafluoroborate fluoboric acid hydrofluoroboric acid	HSDB (1995)
Molecular Formula	HBF ₄	HSDB (1995)
Chemical Structure	B-F ₄ -H	Fisher Scientific (1993)
Physical State	colorless liquid	HSDB (1995)
Molecular Weight	87.82	HSDB (1995)
Melting Point	-90°C	Fisher Scientific (1993)
Boiling Point	130°C (decomposes)	HSDB (1995)
Water Solubility	miscible; sol. in hot water	HSDB (1995)
Density	~1.84 g/mL	HSDB (1995)
K _{oc}	NA	
Log K _{ow}	NA	
Vapor Pressure	5.1 mm Hg at 20°C	Fisher Scientific (1993)
Vapor Density	3.0	Fisher Scientific (1993)
Reactivity	strong acid; corrosive	HSDB (1995)
Flammability	NA	
Flash Point	NA	
Dissociation Constant (-pK)	-4.9	HSDB (1995)
Henry's Law Constant	NA	
Molecular Diffusivity Coefficient	NA	
Air Diffusivity Coefficient	NA	
Fish Bioconcentration Factor	NA	
Odor Threshold	NA	
Conversion Factors	Na	

The chemical identity and physical/chemical properties of sodium tetrafluoroborate are summarized in Table 2.

TABLE 2. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM TETRAFLUOROBORATE

Characteristic/Property	Data	Reference
CAS No.	013755-29-8	Lockheed Martin (1994)
Common Synonyms	sodium fluoroborate STB sodium borfluoride sodium boron tetrafluoride	Lockheed Martin (1994)
Molecular Formula	NaNF ₄	
Chemical Structure	Na-F ₄ -B	
Physical State	white crystalline powder	Sigma-Aldrich (1992)
Molecular Weight	109.82	Budavari et al. (1989)
Melting Point	384 °C	Budavari et al. (1989)
Boiling Point		
Water Solubility	108 g/100 mL at 26 °C 210 g/100 mL at 100 °C	Budavari et al. (1989)
Density	2.470	Sigma-Aldrich (1992)
K _{OC}	NA	
Log K _{OW}	NA	
Vapor Pressure	NA	
Reactivity	reacts with strong oxidizing agents; sensitive to moisture	Sigma-Aldrich (1992)
Flammability	noncombustible	Lockheed Martin (1994)
Flash Point	NA	
Dissociation Constant (-pK)		
Henry's Law Constant		
Molecular Diffusivity Coefficient	NA	
Air Diffusivity Coefficient	NA	
Fish Bioconcentration Factor	NA	
Odor Threshold	NA	
Conversion Factors	NA	

The chemical identity and physical/chemical properties of sodium fluoride are summarized in Table 3.

TABLE 3. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM FLUORIDE

Characteristic/Property	Data	Reference
CAS No.	7681-49-4	
Common Synonyms	sodium hydrofluoride sodium monfluoride floridine	
Molecular Formula	NaF	
Chemical Structure	Na-F	
Physical State	crystals	Budavari et al. (1989)
Molecular Weight	42.00	Budavari et al. (1989)
Melting Point	993 °C	Budavari et al. (1989)
Boiling Point	1704 °C	Budavari et al. (1989)
Water Solubility	4.0 g/100 mL at 15 °C 4.3 g/100 mL at 25 °C	Budavari et al. (1989)
Density	2.78	Budavari et al. (1989)
K _{oc}	NA	
Log K _{ow}	NA	
Vapor Pressure	1 mm Hg at 1077 °C	Keith and Walters (1985)
Reactivity	stable under normal conditions	Keith and Walters (1985)
Flammability	nonflammable	Keith and Walters (1985)
Flash Point		
Dissociation Constant (-pK)		
Henry's Law Constant		
Molecular Diffusivity Coefficient		
Air Diffusivity Coefficient		
Fish Bioconcentration Factor		
Odor Threshold		
Conversion Factors		

The chemical identity and physical/chemical properties of sodium bifluoride are summarized in Table 4.

TABLE 4. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM BIFLUORIDE

Characteristic/Property	Data	Reference
CAS No.	1333-83-1	HSDB (1995)
Common Synonyms	sodium hydrogen difluoride sodium hydrogen fluoride sodium acid fluoride	HSDB (1995)
Molecular Formula	NaHF ₂	Lewis (1993)
Chemical Structure	F ₂ -H-Na	HSDB (1995)
Physical State	white, crystalline powder	Budavari et al. (1989)
Molecular Weight	62.01	Budavari et al. (1989)
Melting Point	decomposes on heating	Lewis (1993)
Boiling Point	NA	
Water Solubility	soluble in cold and hot water	Lide (1991)
Density	2.08	Lewis (1993)
K _{OC}	NA	
Log K _{OW}	NA	
Vapor Pressure	NA	
Vapor Density	NA	
Reactivity	aqueous solution corrodes glass	Budavari et al. (1989)
Flammability	slightly combustible	Lockheed Martin (1990)
Flash Point	NA	
Dissociation Constant (-pK)	NA	
Henry's Law Constant	NA	
Molecular Diffusivity Coefficient	NA	
Air Diffusivity Coefficient	NA	
Fish Bioconcentration Factor	NA	
Odor Threshold	NA	
Conversion Factors	NA	

II. ENVIRONMENTAL FATE

A. Environmental Release

Fluoroboric acid may be released into the environment in emissions and effluents from facilities involved in its manufacture or use. It is used primarily in industrial metal plating solutions (60%), in the synthesis of diazo salts (20%), and in metal finishing (20%) (HSDB 1995). It is used in bright dipping solutions for Sn-Pb alloys in printed circuits and other electrical components (HSDB 1995).

B. Transport

No information was found in the available secondary sources on the environmental transport of fluoroboric acid. Its miscibility with water indicates that transport in aqueous systems is very likely.

C. Transformation/Persistence

FLUOROBORIC ACID:

1. Air — No information was found in the available secondary sources on the transformation and persistence of fluoroboric acid or fluoroborates in the atmosphere.
2. Soil — No information was found in the available secondary sources on the transformation and persistence of fluoroboric acid or fluoroborates in soil. Fluoroboric acid may undergo limited hydrolysis in moist soils (Budavari et al. 1989).
3. Water — Fluoroboric acid undergoes limited hydrolysis in water to form hydroxyfluoroborate ions, the major product is BF_3OH^- (Budavari et al. 1989).
4. Biota — No information was found in the available secondary sources on the biotransformation or bioconcentration of fluoroboric acid or fluoroborates. Rapid urinary excretion of tetrafluoroborates suggests that these salts would not bioaccumulate.

FLUORIDES:

1. Air — Gaseous inorganic fluorides undergo hydrolysis in the atmosphere; however, particulate forms are relatively stable and do not hydrolyze readily (ATSDR 1993).
2. Soil — Fluorides tend to persist in soils as fluorosilicate complexes under acidic conditions and as calcium fluoride under alkaline conditions. Sandy acidic soils favor the formation of soluble forms (ATSDR 1993).
3. Water — In dilute solutions and at neutral pH, fluoride is generally present as dissolved fluoride ion. High calcium carbonate levels may lead to precipitation as calcium fluoride (ATSDR 1993).
4. Biota — Fluorides have been shown to accumulate in some aquatic organisms (ATSDR 1993). Soluble forms of fluoride are taken up by terrestrial plants and converted into fluoro-organic compounds (ATSDR 1993).

CHEMICAL SUMMARY FOR HYDROCHLORIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of hydrochloric acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF HYDROCHLORIC ACID

Characteristic/Property	Data	Reference
CAS No.	7647-01-0	Budavari et al. (1996)
Common Synonyms	muratic acid	Budavari et al. (1996)
Molecular Formula	HCl	Budavari et al. (1996)
Chemical Structure	HCl	Budavari et al. (1996)
Physical State	fuming liquid	Lewis (1993)
Molecular Weight	36.46	Lide (1995)
Melting Point	-25.4 °C (39.17% soln)	Budavari et al. (1996)
Boiling Point	108.58 °C at 760 mm Hg	Budavari et al. (1996)
Water Solubility	479.1 g/l (40% soln)	Weast et al. (1985)
Density	1.20 g/cm ³ (39.11% soln)	Budavari et al. (1996)
Vapor Density (air = 1)	1.639 g/l	Austin and Glowacki (1989)
Koc	expected to be < 50	SRC (1998)
Log Kow	expected to be < 1	SRC (1998)
Vapor Pressure	no data	
Reactivity	toxic, corrosive fumes w/H ₂ O or steam	Sax (1984)
Flammability	non-combustible	Lewis (1993)
Flash Point	no data	
Dissociation Constant	~ -3	Bodek et al. (1988)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data	
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If hydrochloric acid is released into the water column at low concentrations, a pK_a of ~ -3.00 (Bodek et al., 1988) indicates it will dissociate completely into chloride (Cl⁻) and hydrogen (H⁺) ions. The amount of gaseous hydrochloric acid dissolved in water is affected by the pH of the solution. A higher pH allows more aqueous hydrochloric acid to dissociate, thereby increasing the solubility of hydrochloric acid gas (Bodek et al., 1988). As a result, dilute solutions of hydrochloric acid are not expected to volatilize from water surfaces or to bioconcentrate in aquatic organisms. Chloride ions generally do not react with many species in water and are harmless at relatively low concentrations (Manahan, 1991). Hydrochloric acid will protonate amines and other electron pair donors present in

natural waters, forming salts; this will be dependent upon pH. Large releases of the concentrated acid into water, such as may result from a spill, will result in a lowering of the pH (Bodek et al., 1988).

B. Atmospheric Fate

If hydrochloric acid is released to the atmosphere, its vapor pressure indicates it will exist as a vapor in the ambient atmosphere. Wet deposition of hydrochloric acid in rain, snow, or fog is expected to be the dominant fate process in the atmosphere based upon its high water solubility (Arimoto, 1989).

C. Terrestrial Fate

If hydrochloric acid is released to soil, it will dissociate into chloride and hydrogen ions in moist soils. Hydrochloric acid will protonate amines and other electron pair donors present in soils, forming salts; this will be dependent upon pH. The chloride ion is extremely mobile in soils and almost no soil retention occurs (Bodek et al., 1988). Chloride is typically the predominant ion in saline soils and the second most abundant anion in sodic soils; thus, it is readily available for the formation of metal complexes in soil (Bodek et al., 1988; SRC, 1998).

D. Summary

If released into water, hydrochloric acid will dissociate into chloride (Cl^-) and hydrogen (H^+) ions. Therefore, hydrochloric acid is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, nor volatilize from water surfaces. Chloride ions generally do not react with many species in water and are harmless at relatively low concentrations. Hydrochloric acid will protonate amines and other electron pair donors present in natural waters and soils, forming salts; this will be dependent upon pH. If released to soil, hydrochloric acid is expected to dissociate into its component ions in moist soils. Because the chloride ion is extremely mobile in soils, almost no soil retention occurs. Chloride is typically the predominant ion in saline soils and the second most abundant anion in sodic soils; thus, it is readily available for the formation of metal complexes in soil. Volatilization of hydrochloric acid from soil surfaces is not expected to occur. If released to the atmosphere, hydrochloric acid is expected to exist as a gas. Hydrochloric acid is expected to be physically removed from the atmosphere by wet deposition based upon its high water solubility.

CHEMICAL SUMMARY FOR HYDROGEN PEROXIDE

This chemical was identified by one or more suppliers as a bath ingredient for the electroless copper, non-formaldehyde electroless copper, and tin-palladium processes. This summary is based on information retrieved from a systematic search limited to secondary sources (see Attachment C-1). These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of hydrogen peroxide are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF HYDROGEN PEROXIDE

Characteristic/Property	Data	Reference
CAS No.	7722-84-1	
Common Synonyms	hydrogen dioxide; hydroperoxide; albone; hioxyl	Budavari et al. 1989
Molecular Formula	H ₂ O ₂	Budavari et al. 1989
Chemical Structure	H ₂ O ₂	IARC 1985
Physical State	colorless, unstable liquid, bitter taste	Budavari et al. 1989
Molecular Weight	34.02	Budavari et al. 1989
Melting Point	-0.43 °C	Budavari et al. 1989
Boiling Point	152 °C	Budavari et al. 1989
Water Solubility	miscible	Budavari et al. 1989
Density	1.463 @ 0 °C	Budavari et al. 1989
Vapor Density (air = 1)	no data	
K _{oc}	no data	
Log K _{ow}	no data	
Vapor Pressure	1.97 mm Hg @ 25 ° C (measured)	CHEMFATE 1995
Reactivity	strong oxidizer; may decompose violently if traces of impurities are present molecular additions, substitutions, oxidations, reduction; can form free radicals	Budavari et al. 1989 IARC 1985
Flammability	not flammable, but can cause spontaneous combustion of flammable materials	HSDB 1995
Flash Point	no data	
Dissociation Constant	no data	
Henry's Law Constant	no data	
Molecular Diffusivity Coefficient	no data	
Air Diffusivity Coefficient	no data	
Fish Bioconcentration Factor	no data	
Odor Threshold	odorless	Budavari et al. 1989
Conversion Factors	1 ppm = 1.39 mg/m ³ 1 mg/m ³ = 0.72 ppm 30% soln 1.1 kg/L anhydrous 1.46 kg/L	IARC 1985 Budavari et al. 1989

II. ENVIRONMENTAL FATE

A. Environmental Release

No information was found in the secondary sources searched regarding the environmental release of hydrogen peroxide. Solutions of hydrogen peroxide gradually deteriorate (Budavari et al., 1989). Hydrogen peroxide is a naturally occurring substance. Gaseous hydrogen peroxide is recognized to be a key component and product of the earth's lower atmospheric photochemical reactions, in both clean and polluted atmospheres. Atmospheric hydrogen peroxide is also believed to be generated by gas-phase photochemical reactions in the remote troposphere (IARC, 1985)

B. Transport

No information was found in the secondary sources searched regarding the transport of hydrogen peroxide.

C. Transformation/Persistence

1. Air — Hydrogen peroxide may be removed from the atmosphere by photolysis giving rise to hydroxyl radicals, by reaction with hydroxyl radicals, or by heterogenous loss processes such as rain-out (IARC, 1985).
2. Soil — No information was found in the secondary sources searched regarding the transformation or persistence of hydrogen peroxide in soil, however, solutions of hydrogen peroxide gradually deteriorate (Budavari et al., 1989).
3. Water — Hydrogen peroxide is a naturally occurring substance. Surface water concentrations of hydrogen peroxide have been found to vary between 51-231 mg/L, increasing both with exposure to sunlight and the presence of dissolved organic matter (IARC, 1985).
4. Biota — Hydrogen peroxide is a naturally occurring substance. Endogenous hydrogen peroxide has been found in plant tissues at the following levels (mg/kg frozen weight): potato tubers, 7.6; green tomatoes, 3.5; red tomatoes, 3.5; and castor beans in water, 4.7 (IARC, 1985).

CHEMICAL SUMMARY FOR LEAD

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for Lead.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of Lead are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF LEAD

Characteristic/Property	Data	Reference
CAS No.	7439-92-1	Howard and Neal (1992)
Common Synonyms		
Molecular Formula	Pb	Howard and Neal (1992)
Chemical Structure	N/A	
Physical State	Metal	Weast (1983)
Molecular Weight	207.2	Weast (1983)
Melting Point	327.4°C	Weast (1983)
Boiling Point	1740°C	Weast (1983)
Water Solubility	Insoluble	Weast (1983)
Density	10.65	Budavari et al. (1996)
Vapor Density (air = 1)	no data	
Koc	no data	
Log Kow	no data	
Vapor Pressure	1.77 mm Hg @ 1000°C	Budavari et al. (1996)
Reactivity	Flammable solid	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data	
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

CHEMICAL SUMMARY FOR MALEIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of maleic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF MALEIC ACID

Characteristic/Property	Data	Reference
CAS No.	110-16-7	Lide (1995)
Common Synonyms	(Z)-butenedioic acid; toxilic acid	Budavari et al. (1996)
Common Synonyms	cis-1,2-ethylenedicarboxylic acid	Budavari et al. (1996)
Common Synonyms	maleinic acid	Lewis (1993)
Molecular Formula	C ₄ H ₄ O ₄	Budavari et al. (1996)
Chemical Structure	HOOCCH=CHCOOH	Aldrich (1996)
Physical State	white crystals	Budavari et al. (1996)
Molecular Weight	116.07	Budavari et al. (1996)
Melting Point	130.5°C	Lide (1995)
Boiling Point	no data	
Water Solubility	441 g/l at 25 °C	PHYSPROP (1998)
Density	1.59 g/cm ³ at 20 °C	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	16 (estimated)	Lyman et al. (1990)
Log Kow	-0.34	Hansch et al. (1995)
Vapor Pressure	3.06x10 ⁻⁵ mm Hg at 25 °C	Daubert and Danner (1991)
Reactivity	stable	Weiss (1986)
Flammability	combustible	Lewis (1993)
Flash Point	not pertinent	Weiss (1986)
Dissociation Constant	pK ₁ = 1.83; pK ₂ = 6.07	Howard (1989)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; estimated to be < 1x10 ⁻⁸ atm m ³ /mol	Estimated
Fish Bioconcentration Constant	10-11	HSDB (1998)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into water, maleic acid is not expected to adsorb to suspended solids or sediments in water based upon an estimated Koc of 16 (Swann et al., 1983), determined from a log Kow of -0.34 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990). Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990) based on an estimated Henry's Law constant of <10⁻⁸ atm-m³/mole. Maleic acid is expected to be stable to hydrolysis in the pH range of 5-9 typically encountered in the environment (Lyman et

al., 1990). According to a classification scheme (Franke et al., 1994), a BCF of 10 in golden ide fish (Freitag, 1985, as cited in HSDB, 1998) suggests that the potential for bioconcentration in aquatic organisms is low. Maleic acid was determined to be readily degraded in biodegradation screening tests; however, no biodegradation studies were available in environmental waters (Howard, 1989).

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), maleic acid, which has a vapor pressure of 3.06×10^{-5} mm Hg at 25 °C (Daubert and Danner, 1991), is expected to exist as both a particulate and vapor in the ambient atmosphere. Because maleic acid has pKa's of 1.83 and 6.07 (Howard, 1989), it is expected to exist in the dissociated form in the environment and form salts with cations (HSDB, 1998). Removal of maleic acid from the atmosphere by reaction with photochemically-produced hydroxyl radicals results in an estimated half-life of 2 days (Meylan and Howard, 1993). The reaction of maleic acid with ozone in the atmosphere results in a gas-phase half-life ranging from 7-13 days (Meylan and Howard, 1993). Maleic acid may undergo some degradation by direct photolysis; 17% of applied maleic acid was degraded after 17 hours following irradiation by light > 290 nm (Freitag et al., 1985, cited in HSDB, 1998). Wet deposition of maleic in rain, snow, or fog is expected to be an important transport process in the atmosphere based upon its high water solubility (Arimoto, 1989).

C. Terrestrial Fate

Based on a classification scheme (Swann et al., 1983), an estimated Koc of 16, determined from a log Kow of -0.34 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990), indicates that maleic acid is expected to have very high mobility in soil. Volatilization of maleic acid from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an estimated Henry's Law constant of $<10^{-8}$ atm-m³/mole. In addition, maleic acid is not expected to volatilize from dry soil given its vapor pressure of 3.06×10^{-5} mm Hg (Daubert and Danner, 1991). While maleic acid is readily biodegradable in screening studies, no degradation data were available for soil systems (Howard, 1989).

D. Summary

If released to air, a vapor pressure of 3.06×10^{-5} mm Hg at 25 °C indicates that maleic acid should exist as both a gas and particulate in the ambient atmosphere. Gas-phase maleic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 2 hours. The reaction of maleic acid with ozone in the atmosphere results in a gas-phase half-life ranging from 7-13 days. Wet deposition of maleic acid from the atmosphere is expected to be an important transport process. Screening studies suggest that direct photolysis of maleic acid may occur. A BCF of 10 in golden ide fish suggests the potential for bioconcentration in aquatic organisms is low. If released to soil, maleic acid is expected to have very high mobility based upon an estimated Koc of 16, and, therefore, it has the potential to leach to groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of $<10^{-8}$ atm-m³/mole. Volatilization from dry soil surfaces is not expected to occur based upon the vapor pressure of this compound. Maleic acid was determined to be readily biodegraded in screening studies, although no data were available for biodegradation in water or soil.

CHEMICAL SUMMARY FOR MALIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of malic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF MALIC ACID

Characteristic/Property	Data	Reference
CAS No.	6915-15-7	Lewis (1993)
Common Synonyms	hydroxysuccinic acid; apple acid	Lewis (1993)
Molecular Formula	C ₄ H ₆ O ₅	Budavari et al. (1996)
Chemical Structure	COOHCH ₂ CH(OH)COOH	Lewis (1993)
Physical State	colorless crystals	Lewis (1993)
Molecular Weight	134.09	Budavari et al. (1996)
Melting Point	100 °C	Budavari et al. (1996)
Boiling Point	140 °C, decomposes	Budavari et al. (1996)
Water Solubility	592 g/l at 25 °C	PHYSPROP (1998)
Density	1.6 g/cm ³	Lewis (1993)
Vapor Density (air = 1)	no data	
Koc	5 (estimated)	Lyman et al. (1990)
Log Kow	-1.26	Hansch et al. (1995)
Vapor Pressure	3.28x10 ⁻⁸ mm Hg at 25 °C	Yaws (1994)
Reactivity	no data	
Flammability	combustible	Lewis (1993)
Flash Point	no data	
Dissociation Constant	3.40	PHYSPROP (1998)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be < 10 ⁻⁸ atm m ³ /mol	Estimated
Fish Bioconcentration Constant	no data; expected to be <1	Estimated
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into aquatic waters, malic acid is not expected to adsorb to suspended solids and sediments in water based upon an estimated Koc of 5 (Swann et al., 1983), determined from a log Kow of -1.26 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990). Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990) based on an estimated Henry's Law constant of <10⁻⁸ atm-m³/mole. Malic acid is expected to be stable to hydrolysis in the pH range of 5-9 typically encountered in the environment (Lyman et al., 1990). According to a classification scheme (Franke et al., 1994), an estimated BCF of <1 suggests that the potential for bioconcentration in aquatic organisms is low and not an important fate process. Results from a number

of biological screening tests have shown that malic acid biodegrades relatively fast (Fischer et al., 1974; Malaney and Gerhold, 1969; Heukelekian and Rand, 1955; as cited in HSDB, 1998).

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), malic acid, which has a vapor pressure of 3.28×10^{-8} mm Hg at 25 °C (Yaws, 1994), should exist almost entirely as a particulate in the ambient atmosphere. Removal of malic acid from the atmosphere by reaction with photochemically-produced hydroxyl radicals results in an estimated half-life of 2 days (Meylan and Howard, 1993). Wet deposition of malic acid in rain, snow, or fog is expected to be the dominant transport process in the atmosphere based upon its high water solubility (Arimoto, 1989). Because carboxylic acids are generally resistant to hydrolysis, malic acid is not expected to hydrolyze in environmental media (Lyman et al., 1990).

C. Terrestrial Fate

Based on a classification scheme (Swann et al., 1983), an estimated Koc of 5, determined from a log Kow of -1.26 (Hansch et al., 1995) and a regression-derived equation (Lyman et al., 1990), indicates that malic acid is expected to have very high mobility in soil and may leach to groundwater. Volatilization of malic acid from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an estimated Henry's Law constant of $<10^{-8}$ atm-m³/mole. In addition, malic acid is not expected to volatilize from dry soil given its vapor pressure of 3.28×10^{-8} mm Hg (Yaws, 1994). Biodegradation screening studies reveal that malic acid biodegrades relatively fast (Fischer et al., 1974; Malaney and Gerhold, 1969; Heukelekian and Rand, 1955; as cited in HSDB, 1998).

D. Summary

If released to air, a vapor pressure of 3.28×10^{-8} mm Hg at 25 °C indicates that malic acid should exist as a particulate in the ambient atmosphere. Removal of malic acid from the atmosphere by reaction with photochemically-produced hydroxyl radicals results in an estimated half-life of 2 days. Wet deposition is expected to be the dominant transport process of malic acid from the atmosphere. An estimated BCF of <1 suggests the potential for bioconcentration in aquatic organisms is low. If released to soil, malic acid is expected to have very high mobility based upon an estimated Koc of 5, and, therefore, it has the potential to leach to groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of $<10^{-8}$ atm-m³/mole, also volatilization from dry soil surfaces is not expected to occur based upon the vapor pressure of this compound. Hydrolysis of malic acid in environmental media is not expected to occur. Malic acid was determined to be readily biodegraded in screening studies, although no data were available for biodegradation in water or soil.

CHEMICAL SUMMARY FOR METHANESULFONIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of methanesulfonic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF METHANESULFONIC ACID

Characteristic/Property	Data	Reference
CAS No.	75-75-2	Lide (1995)
Common Synonyms	methylsulfonic acid	Budavari et al. (1996)
Molecular Formula	CH ₄ O ₃ S	Budavari et al. (1996)
Chemical Structure	CH ₃ SO ₂ OH	Budavari et al. (1996)
Physical State	solid	Budavari et al. (1996)
Physical State	liquid at room temperature	Lewis (1993)
Molecular Weight	96.11	Budavari et al. (1996)
Melting Point	20 °C	Lide (1995)
Boiling Point	200 °C; 167 °C at 10 mm Hg	Lewis (1993); Lide (1995)
Water Solubility	1.0x10 ³ g/L at 20 °C	PHYSPROP (1998)
Density	1.48 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	1 (estimated)	HSDB (1998)
Log Kow	no data; estimated to be < 1	Estimated
Vapor Pressure	4.28x10 ⁻⁴ mm Hg at 25 °C	Daubert and Danner (1991)
Reactivity	thermally stable at mod. elevated temps	Budavari et al. (1996)
Flammability	no data	
Flash Point	112 °C	ECDIN (1998)
Dissociation Constant	-1.86	Serjeant and Dempsey (1979)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	1.3x10 ⁻⁸ atm m ³ /mol (estimated)	Meylan and Howard (1991)
Fish Bioconcentration Constant	3 (estimated)	Meylan et al. (1997)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into aquatic waters, methanesulfonic acid is not expected to adsorb to suspended solids and sediments in water based upon an estimated Koc of 1 (Swann et al., 1983), determined from a structure fragment estimation method (Meylan et al., 1992). Volatilization from the water column to the atmosphere is not expected to occur (Lyman et al., 1990) based on an estimated Henry's Law constant of 1.3x10⁻⁸ atm-m³/mole (Meylan and Howard, 1991; SRC, 1998). Methanesulfonic acid is expected to be stable to hydrolysis in the pH range of 5-9 typically

encountered in the environment (Lyman et al., 1990). According to a classification scheme (Franke et al., 1994), an estimated BCF of 3 (Meylan et al., 1997) suggests that the potential for bioconcentration in aquatic organisms is low. It was determined that many bacterial types can degrade methanesulfonic acid through diverse routes and at different rates, although specifics were not given (Baker et al., 1991, as cited in HSDB, 1998). Because methanesulfonic acid has pKa of -1.86 (Serjeant and Dempsey, 1979), it is expected to exist in the dissociated form in the environment.

B. Atmospheric Fate

According to a model of gas/particle partitioning of semivolatile organic compounds in the atmosphere (Bidleman, 1988), methanesulfonic acid, which has a vapor pressure of 4.28×10^{-4} mm Hg at 25 °C (Daubert and Danner, 1991), has the potential to exist as both a vapor and particulate in the ambient atmosphere. Because methanesulfonic acid has pKa of -1.86 (Serjeant and Dempsey, 1979), it is expected to exist in the dissociated form in the environment. Removal of methanesulfonic acid from the atmosphere by reaction with photochemically-produced hydroxyl radicals results in an estimated half-life of 58 days (Meylan and Howard, 1993). In the atmosphere, methanesulfonic acid is concentrated in the smaller size particles, 0.25-2 μ m in diameter (Kolaitis et al., 1989, as cited in HSDB, 1998). Removal of particulate methanesulfonic acid from the atmosphere can occur through wet and dry deposition (HSDB, 1998).

C. Terrestrial Fate

Based on a classification scheme (Swann et al., 1983), an estimated Koc of 1, determined from a structure fragment estimation method (Meylan et al., 1992), indicates that methanesulfonic acid is expected to have very high mobility in soil. Volatilization of methanesulfonic acid from moist soil surfaces is not expected to be important (Lyman et al., 1990) given an estimated Henry's Law constant of 1.3×10^{-8} atm-m³/mole (Meylan and Howard, 1991; SRC, 1998). In addition, methanesulfonic acid is not expected to volatilize from dry soil given its vapor pressure of 4.28×10^{-4} mm Hg (Daubert and Danner, 1991). It was determined that many bacterial types can degrade methanesulfonic acid through diverse routes and at different rates, although specifics were not given (Baker et al., 1991, as cited in HSDB, 1998).

D. Summary

If released to air, a vapor pressure of 4.28×10^{-4} mm Hg at 25 °C indicates that methanesulfonic acid has the potential to exist as both a vapor and particulate in the ambient atmosphere. Gas-phase methanesulfonic acid will be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air is estimated to be 58 hours. Removal of particulate methanesulfonic acid from the atmosphere can occur through wet and dry deposition. An estimated BCF of 3 suggests the potential for bioconcentration in aquatic organisms is low. If released to soil, methanesulfonic acid is expected to have very high mobility based upon an estimated Koc of 1, and, therefore, it has the potential to leach to groundwater. Volatilization from water and from moist soil surfaces is not expected to be an important fate process based upon an estimated Henry's Law constant of 1.3×10^{-8} atm-m³/mole. Hydrolysis of methanesulfonic acid is not expected to occur. Volatilization from dry soil surfaces is not expected to occur based upon the vapor pressure of this compound. Methanesulfonic acid was determined to be biodegraded by many bacterial types, although specifics were not given.

CHEMICAL SUMMARY FOR NICKEL SULFATE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for nickel and soluble salts of nickel, including nickel sulfate and nickel sulfate hexahydrate.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of nickel sulfate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF NICKEL SULFATE

Characteristic/Property	Data	Reference
CAS No.	7786-81-4	Lide (1995)
Common Synonyms	sulfuric acid, nickel (2+) salt	Howard and Neal (1992)
Molecular Formula	NiO ₄ S	Budavari et al. (1996)
Chemical Structure	NiSO ₄	Lide (1995)
Physical State	green-yellow orthorhombic crystals	Lide (1995)
Molecular Weight	154.757	Lide (1995)
Melting Point	840 °C, decomposes	Lide (1995)
Boiling Point	no data	
Water Solubility	293 g/L at 0 °C	Dean (1985)
Density	4.01 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be < 10	SRC (1998)
Log Kow	no data; expected to be < 1	SRC (1998)
Vapor Pressure	no data; expected to be <10-6 mm Hg at 25 C	Estimated
Reactivity	no data	
Flammability	not flammable	Prager (1995)
Flash Point	no data; expected to be > 350 °C	SRC (1998)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be < 1x10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released into water, nickel sulfate is expected to dissociate into nickel (Ni²⁺) and sulfate [(SO₄)²⁻] ions. The dissociation of nickel sulfate into its component ions indicates that the compound nickel sulfate is not expected to volatilize from water surfaces. In aqueous solutions, nickel exists as the hexaquonickel ion, [Ni(H₂O)₆²⁺]; this ion is poorly absorbed by most living organisms (Sunderman and Oskarsson, 1991). In natural waters, nickel exists both in the ionic form and as stable organic complexes (Sunderman and Oskarsson, 1991). Nickel compounds are generally

soluble at pH values less than 6.5, but at pH values greater than 6.7 nickel exists predominantly as insoluble nickel hydroxides (Sunderman and Oskarsson, 1991). Shellfish and crustacea generally contain higher concentrations of nickel in their flesh than do other species of fish (Sunderman and Oskarsson, 1991).

B. Atmospheric Fate

If released to the atmosphere, nickel sulfate's high melting point (Lide, 1995) and low vapor pressure (SRC, 1998) indicate that it will exist as a particulate (Bidleman, 1988). Wet and dry deposition of nickel sulfate is expected to be the dominant fate process in the atmosphere (Arimoto, 1989). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). Nickel sulfate's high water solubility (Dean, 1985) indicates that it is expected to undergo wet deposition in rain, snow, or fog.

C. Terrestrial Fate

If nickel sulfate is released to soil, it is expected to dissociate into Ni^{2+} and $(\text{SO}_4)^{2-}$ ions in the presence of moisture. Iron and manganese oxides, clay minerals, and organic matter may be important sorbents of nickel (Bodek et al., 1988) and will retard its migration through soil. Complexing ligands, such as organic acids, may reduce the sorption of nickel (Bodek et al., 1988). Acid rain has a tendency to mobilize nickel from soil and increase leaching into groundwater due to the high solubility of nickel compounds at pH values less than 6.5 (Sunderman and Oskarsson, 1991). The high melting point, low vapor pressure, and low Henry's Law constant expected for an ionic salt indicate that nickel sulfate will not volatilize from either moist or dry soil surfaces (Bodek et al., 1988).

D. Summary

If released into water, nickel sulfate is expected to dissociate into nickel (Ni^{2+}) and sulfate ($(\text{SO}_4)^{2-}$) ions. Therefore, nickel sulfate is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, or volatilize from water surfaces. In natural waters, nickel exists in both the ionic form and as stable organic complexes; at pH values greater than 6.7 it exists as insoluble nickel hydroxides. In moist soils, nickel sulfate is expected to dissociate into its component ions. Ionic nickel may be sorbed by iron and manganese oxides, clay minerals, and organic matter; acid rain and complexing ligands may reduce the sorption of nickel. Volatilization of nickel sulfate from soil surfaces is not expected to occur. If released to the atmosphere, nickel sulfate is expected to exist as a particulate. Nickel sulfate is expected to be physically removed from the atmosphere by wet and dry deposition. The rate of dry deposition will depend on particle size and prevailing wind patterns.

CHEMICAL SUMMARY FOR PALLADIUM CHLORIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of palladium chloride are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF PALLADIUM CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	7647-10-1	CAS (1998)
Common Synonyms	Palladous chloride	Budavari et al. (1996)
Common Synonyms	Palladium (II) chloride	Lide (1995)
Molecular Formula	Cl ₂ Pd	Budavari et al. (1996)
Chemical Structure	PdCl ₂	Budavari et al. (1996)
Physical State	red rhombohedral crystals; hygroscopic	Lide (1995)
Molecular Weight	177.33	Lide (1995)
Melting Point	500 °C (decomposes)	Lide (1995)
Boiling Point	decomposed at high temperatures	Budavari et al. (1996)
Water Solubility	soluble ¹	Dean (1985)
Density	4.0 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	SRC (1998)
Log Kow	no data; expected to be <1	SRC (1998)
Vapor Pressure	no data; expected to be <10 ⁻⁶ mm Hg	SRC (1998)
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	expected to dissociate into Pd ²⁺ and Cl ⁻	SRC (1998)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ This form of expressing solubility cannot be converted into g/L units

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If palladium chloride is released into the water column, it is expected to dissociate into palladium (Pd²⁺) and chloride (Cl⁻) ions. The dissociation of palladium chloride into its component ions indicates that palladium chloride is not expected to bioconcentrate in aquatic organisms or volatilize from water surfaces. Palladium ions may adsorb to charged surfaces of suspended sediments and humic materials in the water column (Evans, 1989). The chloride ion may complex with heavy metals in natural waters, thereby increasing their solubility (Bodek et al., 1988). Adsorption

of the chloride ion to suspended solids and sediment in the water column is not expected to be an important fate process.

B. Atmospheric Fate

If palladium chloride is released to the atmosphere, the low vapor pressure expected for an ionic salt indicates that it will exist as a particulate. Dry deposition of palladium chloride is expected to be the dominant fate process in the atmosphere (Arimoto, 1989). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). Palladium chloride is expected to undergo wet deposition (Arimoto, 1989) in rain, snow, or fog, based upon its water solubility (Dean, 1985).

C. Terrestrial Fate

If palladium chloride is released to soil, it is expected to dissociate into its component ions in moist soils. The dissociation of palladium chloride in moist soils indicates that palladium chloride is not expected to volatilize from moist soil surfaces. While no specific information concerning the sorption of ionic palladium in soils was available, some metals adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces (Evans, 1989). If this occurs with palladium then its rate of migration through soil may be slow. Chloride is extremely mobile in soils (Bodek et al., 1988). The chloride ion may complex with heavy metals, thereby increasing their solubility (Bodek et al., 1988) and potential for leaching into groundwater. The low vapor pressure expected for an ionic salt indicates that palladium chloride will not volatilize from dry soil surfaces.

D. Summary

If released into water, palladium chloride will dissociate into palladium and chloride ions. Therefore, palladium chloride is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, nor volatilize from water surfaces. Palladium ions may adsorb to charged surfaces of suspended sediments and humic matter in the water column. Adsorption of the chloride ion to suspended solids and sediment in the water column is not expected to be an important fate process. If released to soil, palladium chloride is expected to dissociate into its component ions in moist soils. The dissociation of palladium chloride into its component ions indicates that palladium chloride is not expected to volatilize from moist soil surfaces. Ionic palladium may adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces. Chloride is extremely mobile in soils. The low vapor pressure expected for an ionic salt indicates that volatilization of palladium chloride from soil surfaces is not expected to be an important fate process. If released to the atmosphere, palladium chloride is expected to exist as a particulate. Palladium chloride is expected to be physically removed from the atmosphere by wet and dry deposition. The rate of dry deposition will depend on particle size and prevailing wind patterns.

CHEMICAL SUMMARY FOR PHOSPHORIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of phosphoric acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF PHOSPHORIC ACID

Characteristic/Property	Data	Reference
CAS No.	7664-38-2	Lide (1995)
Common Synonyms	orthophosphoric acid	Budavari et al. (1996)
Molecular Formula	H ₃ O ₄ P	Budavari et al. (1996)
Chemical Structure	H ₃ PO ₄	Budavari et al. (1996)
Physical State	unstable, orthorhombic crystals; clear, syrupy liquid	Budavari et al. (1996)
Molecular Weight	98.00	Budavari et al. (1996)
Melting Point	42.35 °C (crystals); -11.8 °C (30% soln)	Gard (1996)
Boiling Point	261 °C (crystals); 101.8 °C (30% soln)	Gard (1996)
Water Solubility	5,480 g/l at 20 °C (crystals); 354.1 g/l at 20 °C (30% soln)	Weast et al. (1985)
Density	1.86 g/cm ³ at 25 °C (crystals); 1.18 g/cm ³ at 25 °C (30% soln)	Gard (1996)
Vapor Density (air = 1)	no data	
Koc	expected to be < 10	SRC (1998)
Log Kow	expected to be < 1	SRC (1998)
Vapor Pressure	0.03 mm Hg at 20 °C (crystals); 16.3 mm Hg at 20 °C (30% soln)	Gard (1996)
Reactivity	relatively unreactive at room temperature	Gard (1996)
Flammability	no data	
Flash Point	no data	
Dissociation Constant	pK ₁ : 2.15; pK ₂ : 7.09; pK ₃ : 12.32	Budavari et al. (1996)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	expected to be < 1x10 ⁻⁸ atm m ³ /mole	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Phosphoric acid is a weak tribasic acid with a pK₁ of 2.15 (Budavari et al., 1996) and, if released into the water column at low concentrations, it will dissociate into dihydrogen phosphate (H₂PO₄) and hydrogen (H⁺) ions. Dihydrogen phosphate then dissociates into hydrogen phosphate ion (HPO₄²⁻; pK₂ of 7.09) and orthophosphate ion (PO₄³⁻; pK₃ of 12.32). As a result, phosphoric acid is not expected to volatilize or bioconcentrate in aquatic organisms. The phosphates become available in the water column and form salts, thus affecting biological

productivity (Bodek et al., 1988). Phosphorous, in the form of phosphate, is an essential nutrient to plants in aquatic environments (Bodek et al., 1988). In addition, the phosphates can complex with metal ions in sediment and water to form insoluble species such as FePO_4 and CaHPO_4 (Bodek et al., 1988).

B. Atmospheric Fate

If phosphoric acid is released to the atmosphere, its vapor pressure indicates it will exist predominantly as a vapor in the ambient atmosphere. Wet deposition of phosphoric acid in rain, snow, or fog is expected to be the dominant fate process in the atmosphere based upon its solubility in water (Arimoto, 1989).

C. Terrestrial Fate

If phosphoric acid is released to soil, it will dissociate into dihydrogen phosphate and hydrogen ions, ultimately dissociating to the orthophosphate ion at high pH's. Phosphate added to soil as fertilizer is quickly sorbed and later "fixed" (probably precipitated) into less soluble forms (Bodek et al., 1988). A similar fate is anticipated for phosphate species from phosphoric acid. While the exact mechanism of sorption is uncertain, phosphate fixation is appreciable in all but very coarse-textured soils; only about one-fourth of the fertilizer phosphate is usable by plants, the rest being lost to the occluded soil fraction (Bodek et al., 1988). Phosphorous, in the form of phosphate, is an essential nutrient to plants (Bodek et al., 1988).

D. Summary

Phosphoric acid is a tribasic acid in which the first hydrogen is strongly ionizing, the second moderately weak, and the third very weak. Both acidic and basic salts can be formed from phosphoric acid. If released into water, phosphoric acid will dissociate into dihydrogen phosphate (H_2PO_4) and hydrogen (H^+) ions, eventually dissociating into the orthophosphate ion (PO_4^{3-}) under the proper conditions. Therefore, phosphoric acid is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, nor volatilize from water surfaces. The phosphates become available in the water column and form salts, affecting biological productivity, and complexing with metal ions form insoluble species such as FePO_4 and CaHPO_4 . If released to soil, phosphoric acid is expected to dissociate into its component ions in moist soils. Phosphate added to soil as fertilizer is quickly sorbed and later "fixed" into less soluble forms; phosphate fixation is appreciable in all but very coarse-textured soils; only about one-fourth of the fertilizer phosphate is usable by plants, the rest being lost to the occluded soil fraction. Phosphorous, in the form of phosphate, is an essential nutrient for aquatic and terrestrial plants. Volatilization of phosphoric acid from soil surfaces is not expected to occur. If released to the atmosphere, phosphoric acid is expected to exist as a gas. Phosphoric acid is expected to be physically removed from the atmosphere by wet deposition based upon its water solubility.

CHEMICAL SUMMARY FOR POTASSIUM AUROCYANIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of potassium aurocyanide are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF POTASSIUM AUROCYANIDE¹

Characteristic/Property	Data	Reference
CAS No. (deleted)	554-07-4	CAS (1998)
CAS No.	13967-50-5	CAS (1998)
Common Synonyms	gold potassium cyanide	Budavari et al. (1996)
Common Synonyms	potassium dicyanoaurate(I)	Budavari et al. (1996)
Molecular Formula	C ₂ AuKN ₂	Budavari et al. (1996)
Chemical Structure	KAu(CN) ₂	Budavari et al. (1996)
Physical State	dihydrate, crystalline powder	Budavari et al. (1996)
Molecular Weight	288.13	Budavari et al. (1996)
Melting Point	no data; expected to be > 350 °C	SRC (1998)
Boiling Point	no data; expected to be > 500 °C	SRC (1998)
Water Solubility	Approximately 130 g/L ²	Budavari et al. (1996)
Water Solubility	1 g dissolves in 0.5 ml boiling H ₂ O	Budavari et al. (1996)
Density	3.45 g/cm ³	Weast (1986)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be < 10	SRC (1998)
Log Kow	no data; expected to be < 1	SRC (1998)
Vapor Pressure	no data; expected to be <10-6 mm Hg at 25 C	SRC (1998)
Reactivity	stable in aqueous solution ²	Cotton and Wilkinson (1966)
Flammability	not flammable	ECDIN (1998)
Flash Point	no data; expected to be > 350 °C	SRC (1998)
Dissociation Constant	readily dissociates to K ⁺ and [Au(CN) ₂] ⁻	Cohn and Stern (1994)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be < 1x10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ Both electrochemical and electroless gold plating processes that use potassium aurocyanide under basic conditions may contain potassium cyanide as a complexing agent (Gmelin, 1998; Cohn and Stern, 1994; McDermott, 1974). The concentration of KCN is typically approximately 6 g/L (0.1 M), although values as high as 200 g/L (3 M) have been reported (Gmelin, 1988).

² Estimated from a reported solubility of 1 g dissolves in 7 ml H₂O (Budavari et al., 1996).

³ Potassium aurocyanide is stable in aqueous solution under both basic and neutral conditions (Cotton and Wilkinson, 1966; Cohn and Stern, 1994). It is also stable in aqueous solutions under acidic conditions (Cohn and Stern, 1994), although common acids such as HCl, H₂SO₄, HNO₃, and H₂S are known to degrade potassium aurocyanide (Gmelin, 1998) and release HCN and gold monocyanoaurate (Budavari et al., 1996; Gmelin, 1998). Concentrated acids and elevated temperatures, or both, are required (Gmelin, 1998). Potassium aurocyanide is commonly used in warm (35-55°C) acidic plating solutions at a pH of approximately 4 (Gmelin, 1998) and stabilized acidic plating baths containing

potassium aurocyanide have been reported down to a pH of 1.5 (McDermott, 1974), yet it is generally considered stable in water above pH 3 (Renner and Johns, 1989). These data indicate that potassium aurocyanide is expected to be chemically stable in the pH range 5-9 typically found in the environment (Lyman et al, 1990), but not under highly acidic conditions such as those found in the stomach (pH 1-2).

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If released to water, potassium aurocyanide will rapidly and completely dissociate into potassium (K^+) and aurocyanide ($[Au(CN)_2]^-$) ions (Cohn and Stern, 1994). The aurocyanide ion is expected to be stable to hydrolysis in the pH range of 5-9 typically encountered in the environment (Lyman et al, 1990; SRC, 1998). The dissociation of potassium aurocyanide into its component ions also indicates that it is not expected to volatilize from water surfaces to the atmosphere, adsorb to sediment and suspended organic matter, or bioconcentrate in fish and aquatic organisms (Bodek et al., 1988).

B. Atmospheric Fate

If released to the atmosphere, potassium aurocyanide will exist as a particulate. Its atmospheric fate will be dominated by deposition to the Earth's surface via wet and dry processes, as potassium aurocyanide is not expected to undergo degradation by the most common atmospheric oxidant, hydroxyl radicals (Lyman et al, 1990; SRC, 1998). The rate of dry deposition will be dependent on the prevailing winds and particle size; fine particles of potassium aurocyanide have the potential to be transported significant distances from their original point of release (Bodek et al, 1988). Potassium aurocyanide is expected to undergo efficient wet deposition in either rain or fog due to its water solubility. Dissolution in clouds followed by wet deposition may also occur. Potassium aurocyanide is stable to light (Cohn and Stern, 1994), and is not expected to undergo degradation by direct photolysis.

C. Terrestrial Fate

If potassium aurocyanide is released to soil, it is expected to display very high mobility based on its water solubility of 143 g/L (Budavari, 1996). Therefore, it has the potential to leach into groundwater. Its rate of leaching through soil may be attenuated by the formation of insoluble soil/aurocyanide complexes that can arise from reactions with metals naturally present in soil (Bodek et al, 1988). The importance of complex formation for potassium aurocyanide in soil is not known. The very high melting point and low vapor pressure expected for an ionic salt indicates that potassium aurocyanide will not volatilize from either moist or dry soils to the atmosphere (Bodek et al, 1988).

D. Summary

If released to water, potassium aurocyanide will dissociate into K^+ and $[Au(CN)_2]^-$ ions. Therefore, it is not expected to adsorb to sediment and suspended organic matter, bioconcentrate in fish and aquatic organisms, or volatilize from water surfaces to the atmosphere. The aurocyanide ion is expected to be chemically stable and it is not expected to hydrolyze in the pH range 5-9 typically found in the environment. In soil, potassium aurocyanide is likely to display very high mobility as a result of its relatively high water solubility and it has the potential to leach to groundwater. Its rate of leaching through soil may be attenuated by the formation of insoluble soil/aurocyanide complexes although the importance of this process is not known. Volatilization from soil surfaces to the atmosphere is not expected to occur. If released to the atmosphere, potassium aurocyanide is expected to exist as a particulate. Its atmospheric fate is expected to be dominated by wet and dry deposition to the Earth's surface. Efficient removal from the atmosphere during rain events is expected although the rate of dry deposition will be dependent on its particle size and the prevailing wind patterns. Therefore, fine particles of potassium aurocyanide have the potential to travel significant distances from their original point of release.

CHEMICAL SUMMARY FOR POTASSIUM PEROXYMONOSULFATE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of potassium peroxymonosulfate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF POTASSIUM PEROXYMONOSULFATE

Characteristic/Property	Data	Reference
CAS No.	10058-23-8	CAS (1998)
Common Synonyms	Monopotassium peroxymonosulfate	Howard and Neal (1992)
Common Synonyms	Peroxymonosulfuric acid, monopotassium salt	Howard and Neal (1992)
Molecular Formula	HO ₅ S.K	Howard and Neal (1992)
Chemical Structure	HOOS(O)(O)OK	CAS (1998)
Physical State	no data	
Molecular Weight	153.18	Howard and Neal (1992)
Melting Point	no data	
Boiling Point	no data	
Water Solubility	no data	
Density	no data	
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	Estimated
Log Kow	no data; expected to be <1	Estimated
Vapor Pressure	no data; expected to be <1X10 ⁻⁶ mm Hg	Estimated
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	expected to dissociate	Bodek et al. (1988)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Most potassium salts are highly dissociated in natural waters (Bodek et al., 1988). Therefore, if potassium peroxymonosulfate is released into water, it is expected to dissociate into potassium (K⁺) and peroxymonosulfate (SO₅⁻) ions. The potassium ion is expected to exist predominately as the free ion in most natural waters (Bodek et al., 1988). Ion exchange processes with suspended solids and sediment in the water column are expected to remove ionic potassium from solution; however, ionic potassium may be displaced by other cations present in natural waters with a

higher affinity for ion exchange sites (Bodek et al., 1988). Aqueous solutions of the impure potassium peroxymonosulfate, i.e., those containing dipotassium sulfate and monopotassium sulfate, decompose yielding mainly O_2 and sulfate (SO_4^{2-}), hydrogen peroxide and peroxydisulfate ($S_2O_8^{2-}$) occur in small amounts (Cotton and Wilkinson, 1980). Sulfate ions may participate in oxidation-reduction reactions or react with cations present in the water column to form soluble complexes or insoluble precipitates (Bodek et al., 1988). Sulfate-reducing microorganisms are important mediators in redox reactions involving this ion (Bodek et al., 1988). Peroxy compounds are short-lived because of the inherent instability of the O-O bond and are expected to degrade rapidly (U.S. EPA, 1993).

B. Atmospheric Fate

If potassium peroxymonosulfate is released to the atmosphere, the low vapor pressure expected for an ionic salt indicates that potassium peroxymonosulfate will exist as a particulate. Wet and dry deposition of potassium peroxymonosulfate is expected to be an important fate process in the atmosphere (Arimoto, 1989). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988).

C. Terrestrial Fate

If potassium peroxymonosulfate is released to soil, it may decompose in moist soils; the importance of this process is not known. The low vapor pressure expected for an ionic salt indicates that potassium peroxymonosulfate will not volatilize from dry soil surfaces. The uncomplexed potassium ion is expected to be the predominant species in well-drained soils from pH 4 to pH 10 (Bodek et al., 1988). Ion exchange reactions are expected to attenuate the mobility of the potassium ion in the subsurface environment, however ionic potassium may be displaced by other cations with a higher affinity for ion exchange sites (Bodek et al., 1988). Peroxy compounds are short-lived because of the inherent instability of the O-O bond and are expected to degrade rapidly (U.S. EPA, 1993).

D. Summary

If released into water, potassium peroxymonosulfate is expected to dissociate into potassium and peroxymonosulfate ions. The dissociation of potassium peroxymonosulfate into its component ions indicates that potassium peroxymonosulfate is not expected to volatilize from water surfaces or bioconcentrate in aquatic organisms. In most natural waters, the potassium ion is expected to exist predominately as the free ion. Ion exchange processes with suspended solids and sediment in the water column are expected to remove ionic potassium from solution; however ionic potassium may be displaced by other cations in natural waters with a higher affinity for ion exchange sites. Sulfate ions may participate in oxidation-reduction reactions or react with cations present in the water column to form soluble complexes or insoluble precipitates; sulfate-reducing microorganisms are important mediators in redox reactions involving this ion. If released to soil, potassium peroxymonosulfate may decompose in moist soils or dissociate into its component ions. As a result, potassium peroxymonosulfate is not expected to volatilize from moist soil surfaces. The low vapor pressure expected for an ionic salt indicates that potassium peroxymonosulfate is not expected to volatilize from dry soil surfaces. The mobility of potassium ions will be retarded by ion exchange processes with charged surfaces of soil particles. However, since the potassium ion is held weakly by ion exchange processes, it may leach into groundwater. Peroxy compounds are short-lived because of the inherent instability of the O-O bond and are expected to degrade rapidly. If released to the atmosphere, potassium peroxymonosulfate is expected to exist as a particulate based upon the low vapor pressure expected for an ionic salt. Wet and dry deposition is expected to be the dominant fate process in the atmosphere.

CHEMICAL SUMMARY FOR PROPIONIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of propionic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF PROPIONIC ACID

Characteristic/Property	Data	Reference
CAS No.	79-09-4	Howard and Neal (1992)
Common Synonyms	methyl acetic acid; ethyl formic acid	Budavari et al. (1996)
Molecular Formula	C ₃ H ₆ O ₂	Budavari et al. (1996)
Chemical Structure	CH ₃ CH ₂ COOH	Budavari et al. (1996)
Physical State	oily liquid	Budavari et al. (1996)
Molecular Weight	74.08	Budavari et al. (1996)
Melting Point	-21.5 °C	Budavari et al. (1996)
Boiling Point	141.1 °C	Budavari et al. (1996)
Water Solubility	1x10 ⁺³ g/l @ 25 °C	U.S. EPA (1981)
Density	d ^{25/4} , 0.99336	Budavari et al. (1996)
Vapor Density (air = 1)	no data	
Koc	36 (calculated)	Lyman et al. (1990)
Log Kow	0.33	Hansch et al. (1995)
Vapor Pressure	3.53 mm Hg @ 25 °C	Daubert and Danner (1985)
Reactivity	corrodes steel, metal	Weiss (1986)
Flammability	combustible	Lewis (1993)
Flash Point	136 °F (58 °C), open cup	Budavari et al. (1996)
Dissociation Constant	pKa = 4.88	Serjeant and Dempsey (1979)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	4.45x10 ⁻⁷ atm m ³ /mole @ 25 °C	Butler and Ramchandani (1935)
Fish Bioconcentration Factor	0.02 (calculated)	Lyman et al. (1990)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Aerobic biodegradation is likely to be the most important removal mechanism of propionic acid from aquatic systems (Dias and Alexander, 1971, as cited in HSDB, 1998). With a pKa of 4.88 (Serjeant and Dempsey, 1979), propionic acid and its conjugate base will exist in environmental waters in varying proportions that are pH dependent. Under neutral and alkaline conditions, propionic acid is expected to exist predominantly as its conjugate base, the propionate ion (Lyman et al., 1990). In addition, at a pH of 4.88 propionic acid is 50% dissociated; even under mildly acidic conditions, it will exist predominantly as the conjugate base. In general, organic ions are not expected to volatilize from water or adsorb to particulate matter in water to the degree that would be predicted for their neutral

counterparts. An estimated Koc of 36, determined from a log Kow of 0.33 (Hansch et al., 1995), indicates propionic acid should not partition from the water column to organic matter contained in sediments and suspended solids. Similarly, the Kow indicates that bioconcentration in fish and aquatic organisms is not an important fate process. Propionic acid's Henry's Law constant of 4.45×10^{-7} atm m³/mole (Butler and Ramchandani, 1935) indicates that volatilization of propionic acid from environmental waters should be extremely slow (Lyman et al., 1990). Volatilization will be attenuated depending upon pH and the amount of propionic acid that is dissociated. Since carboxylic acids are generally resistant to aqueous hydrolysis (Lyman et al., 1990), it is not expected to be an important fate process for propionic acid. The direct photolysis (Calvert and Pitts, 1966, as cited in HSDB, 1998) and reaction of propionic acid with photochemically-generated hydroxyl radicals in water (Anbar and Neta, 1967, as cited in HSDB, 1998) are also not expected to be important fate processes.

B. Atmospheric Fate

Based on a vapor pressure of 3.53 mm Hg at 25 °C (Daubert and Danner, 1985, as cited in HSDB, 1998), propionic acid is expected to exist almost entirely in the vapor phase in the ambient atmosphere (Bidleman, 1988). The rate constant for the reaction of propionic acid with photochemically-produced hydroxyl radicals in air has been experimentally determined to be 1.22×10^{-12} cm³/molecule-sec at 25 °C (Daugaut et al., 1988, as cited in HSDB, 1998). This corresponds to an atmospheric half-life of approximately 13 days. Since low molecular weight organic acids have absorption bands at wavelengths well below the environmentally important range of 290 nm, the direct photolysis of propionic acid in air is not expected to be important (Calvert and Pitts, 1966, as cited in HSDB, 1998). Extensive monitoring data (Chapman et al., 1986; Hoffman and Tanner, 1986; Winkeler et al., 1988; Mazurek and Simoneitt, 1986, as cited in HSDB, 1998) has shown that physical removal of propionic acid from the air by wet deposition (rainfall, dissolution in clouds, etc.) may be an important fate process under the appropriate atmospheric conditions.

C. Terrestrial Fate

Biodegradation is likely to be the most important removal mechanism of propionic acid from aerobic soil (Dias and Alexander, 1971, as cited in HSDB, 1998). With a pKa of 4.88 (Serjeant and Dempsey, 1979), propionic acid and its conjugate base will exist in varying proportions that are dependent on the pH of the soil. A Henry's Law Constant of 4.45×10^{-7} atm m³/mole (Butler and Ramchandani, 1935) indicates that volatilization of propionic acid from moist soil should be extremely slow (Lyman et al., 1990). Yet, propionic acid should volatilize rapidly from dry surfaces based upon a vapor pressure of 3.53 mm Hg at 25 °C (Daubert and Danner, 1985, as cited in HSDB, 1998). Volatilization will be attenuated depending upon pH and the amount of propionic acid dissociated. An estimated Koc of 36, determined from a log Kow of 0.33 (Hansch et al., 1995), indicates that propionic acid may be highly mobile in soil (Swann et al., 1983). In addition, monitoring data has shown that propionic acid can leach to groundwater (Stuermer et al., 1982; Burrows and Rowe, 1975; Lema et al., 1988, as cited in HSDB, 1998). Organic ions generally do not volatilize from moist soil surfaces and do not undergo adsorption to the extent of their neutral counterparts, which is consistent with propionic acid's potential for displaying high mobility through soils under conditions where rapid biodegradation does not occur.

D. Summary

With a pKa of 4.88, propionic acid and its conjugate base will exist in environmental media in varying proportions that are pH dependent; under typical environmental conditions, propionic acid will exist predominantly as its conjugate base. A Henry's Law constant of 4.45×10^{-7} atm m³/mole at 25 °C indicates that volatilization of propionic acid from environmental waters and moist soil should be extremely slow. Yet, based on a vapor pressure of 3.53 mm Hg, propionic acid should volatilize rapidly from dry surfaces. However, volatilization of propionic acid will be pH dependent; if propionic acid is dissociated, very little (about 1%) will be available for volatilization. A relatively low estimated Koc indicates that propionic acid should not partition from the water column to organic matter contained in sediments and suspended solids; the Koc also indicates that it should be highly mobile in soil. However, monitoring data has shown that propionic acid has the potential to leach to groundwater under the appropriate conditions. Propionic acid is miscible with water and monitoring data has shown that physical removal from air by wet deposition is an important removal mechanism. Biodegradation is likely to be the most important removal mechanism of propionic acid from aerobic soil and water. In the atmosphere, propionic acid is expected to exist almost entirely in the gas phase and oxidative removal by photochemically-produced hydroxyl radicals has a half-life of 13 days. The

hydrolysis in water, photolysis in air, and bioconcentration in aquatic organisms are not expected to be important fate processes for propionic acid.

CHEMICAL SUMMARY FOR SILVER NITRATE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for silver nitrate, other nitrate salts and silver.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of silver nitrate are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SILVER NITRATE

Characteristic/Property	Data	Reference
CAS No.	7761-88-8	Lide (1995)
Common Synonyms	silver(I)nitrate	Lide (1995)
Molecular Formula	AgNO ₃	Budavari et al. (1996)
Chemical Structure	AgNO ₃	Lide (1995)
Physical State	colorless, rhombohedral crystals	Lide (1995)
Molecular Weight	169.873	Lide (1995)
Melting Point	212 °C	Lide (1995)
Boiling Point	440 °C decomposes	Lide (1995)
Water Solubility	2,500 g/L water	Budavari et al. (1996)
Density	4.35 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be < 10	SRC (1998)
Log Kow	no data; expected to be < 1	SRC (1998)
Vapor Pressure	no data; expected to be <10-6 mm Hg at 25 °C	Estimated
Reactivity	can explode on contact with soot, organics	Renner (1993)
Flammability	not flammable	Prager (1995)
Flash Point	no data; expected to be > 350 °C	SRC (1998)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be < 1X10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If silver nitrate is released into water, it is expected to dissociate into silver (Ag⁺) and nitrate (NO₃⁻) ions. The dissociation of silver nitrate into its component ions indicates that silver nitrate is not expected to volatilize from water surfaces or bioconcentrate in aquatic organisms (Bodek et al., 1988). Ionic silver may form complexes with hydroxide, sulfide ligands, halide ligands, and chelating organics (Bodek et al., 1988). Silver-organic complexes may be important (Bodek et al., 1988). In aquatic systems with high halide concentrations, precipitation of insoluble silver halides may occur (Bodek et al., 1988). Silver ions may sorb to organic matter and sediment that has high

manganese dioxide, iron oxide, and clay content (Bodek et al., 1988). Nitrate is a minor constituent in natural waters, where its concentration is limited by biological reactions that consume it (Bodek et al., 1988). In aquatic systems where nitrogen is a limiting nutrient, high loadings of nitrate into surface waters can cause algal blooms (Bodek et al., 1988). In natural waters with a low nitrate concentration, complexation with transition metals is not expected to be an important process (Bodek et al., 1988).

B. Atmospheric Fate

If released to the atmosphere, silver nitrate's low vapor pressure indicates that it will exist as a particulate (Bidleman, 1988). Wet and dry deposition of silver nitrate is expected to be the dominant fate process in the atmosphere (Arimoto, 1989). Silver nitrate's high water solubility (Budavari et al., 1996) indicates that it is expected to undergo wet deposition in rain, snow, or fog. The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). Pure silver nitrate is not photosensitive (Cappel, 1997); however, trace amounts of organic material promote its photodegradation (Budavari et al., 1996).

C. Terrestrial Fate

If released to soil, silver nitrate is expected to dissociate into its component ions in the presence of moisture. Silver may adsorb to manganese dioxide, iron oxides, clays, and organic matter (Bodek et al., 1988); therefore, its rate of migration through soil may be slow. The high boiling point, low vapor pressure, and low Henry's Law constant expected for an ionic salt (SRC, 1998) indicates that silver nitrate will not volatilize from either moist or dry soil surfaces. Ionic silver may form complexes with hydroxide, sulfide ligands, halide ligands, and chelating organics (Bodek et al., 1988). Nitrate ions may be converted to gaseous N_2 or nitrous oxide (N_2O) by microorganisms under anaerobic conditions or may be assimilated by plants (Bodek et al., 1988). Sorption of nitrate ions by soils is generally insignificant and therefore nitrate ions are expected to leach into groundwater (Bodek et al., 1988).

D. Summary

If released into water, silver nitrate will dissociate into silver and nitrate ions. Therefore, silver nitrate is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, or volatilize from water surfaces. In natural waters, the concentration of nitrate is limited by biological reactions that consume it. High loadings of nitrate into surface waters can cause algal blooms if nitrogen is a limiting nutrient. Silver nitrate is expected to dissociate into its component ions in moist soils, and ionic silver may adsorb to manganese dioxide, iron oxides, and clays. Nitrate is highly mobile in soils and therefore may leach into groundwater. Under anaerobic conditions nitrate may be converted to gaseous N_2 or nitrous oxide by microorganisms. Volatilization of silver nitrate from soil surfaces is not expected to occur. If released to the atmosphere, silver nitrate is expected to exist as a particulate. Silver nitrate is expected to be physically removed from the atmosphere by wet and dry deposition. Dry deposition will depend on particle size and prevailing wind patterns. Pure silver nitrate is not photosensitive and will not degrade in sunlight; trace amounts of organic material promote silver nitrate's photodegradation.

CHEMICAL SUMMARY FOR SODIUM HYDROXIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of sodium hydroxide are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM HYDROXIDE

Characteristic/Property	Data	Reference
CAS No.	1310-73-2	CAS (1998)
Common Synonyms	Caustic soda	Bodek et al. (1988)
Molecular Formula	HNaO	Budavari et al. (1996)
Chemical Structure	NaOH	Budavari et al. (1996)
Physical State	white orthorhombic crystals; hygroscopic	Lide (1995)
Molecular Weight	39.997	Lide (1995)
Melting Point	323°C	Lide (1995)
Boiling Point	1388°C	Lide (1995)
Water Solubility	571.9 g/L	Weast et al. (1985)
Density	2.13 g/cm ³	Lide (1995)
Vapor Density (air = 1)	not pertinent	Weiss (1986)
Koc	no data; expected to be <10	SRC (1998)
Log Kow	no data; expected to be <1	SRC (1998)
Vapor Pressure	no data; expected to be <10 ⁻⁶ mm Hg	Weiss (1986)
Reactivity	when wet, attacks metals such as aluminum, tin, lead, and zinc to produce flammable hydrogen gas	Weiss (1986)
Flammability	not flammable	Weiss (1986)
Flash Point	not flammable	Weiss (1986)
Dissociation Constant	readily dissociates into Na ⁺ and OH ⁻	SRC (1998)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	not pertinent	Weiss (1986)

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If sodium hydroxide is released into water, it will dissociate into sodium (Na⁺) and hydroxide (OH⁻) ions (Bodek et al., 1988). The dissociation of sodium hydroxide into its component ions indicates that sodium hydroxide is not expected to volatilize from water surfaces or bioconcentrate in aquatic organisms. Because it is strongly basic, sodium hydroxide will react with any protic acids to form salts. Hydroxide is the conjugate base of water; protonation of hydroxide produces water. The presence of hydroxide in natural waters is entirely dependent on the pH of the water, but massive amounts of sodium hydroxide may raise the pH of the receiving water. Metals present in natural waters may form complexes with the hydroxide ion; complexes with transition metals will result in

precipitation of the sparingly soluble metal hydroxides (Bodek et al., 1988). The sodium ion is expected to exist predominately as the free ion in most natural waters (Bodek et al., 1988). Ion exchange processes with suspended solids and sediment in the water column are expected to remove ionic sodium from solution; however, sodium binds weakly to ion exchange sites and is expected to be displaced by other cations present in natural waters (Bodek et al., 1988).

B. Atmospheric Fate

If sodium hydroxide is released to the atmosphere, it is expected to exist as a particulate based upon the low vapor pressure expected for this compound. Wet deposition of sodium hydroxide (Arimoto, 1989) in rain, snow, or fog is expected to be the dominant fate process in the atmosphere based upon its high water solubility (Budavari et al., 1996); however, carbon dioxide dissolved in atmospheric water may react with sodium hydroxide to form sodium carbonate.

C. Terrestrial Fate

If sodium hydroxide is released to soil, it is expected to dissociate into its component ions in moist soils and react with any protic acids present in soil to form the sodium salt and water. The low vapor pressure and low Henry's Law constant expected for an ionic salt indicates that sodium hydroxide will not volatilize from either moist or dry soil surfaces. In soil, ion exchange processes are important in retarding the mobility of sodium ions, however they may be replaced by other soil cations since the sodium ion is held weakly by soils (Evans, 1989).

D. Summary

If released into water, sodium hydroxide will dissociate into sodium and hydroxide ions. The dissociation of sodium hydroxide into its component ions indicates that sodium hydroxide is not expected to volatilize from water surfaces or bioconcentrate in aquatic organisms. The hydroxide ion will react with protic acids to form water. Massive amounts of sodium hydroxide may raise the pH of the water. The sodium ion is expected to participate in ion exchange reactions with charged surfaces of suspended sediments and sediment in the water column. If released to soil, sodium hydroxide is expected to dissociate into its component ions in moist soils and react with protic acids to form water. Sodium hydroxide is not expected to volatilize from moist or dry soil surfaces. The mobility of sodium ions will be retarded by ion exchange processes with charged surfaces of soil particles. However, since the sodium ion is held weakly by ion exchange processes, it may leach into groundwater. If released to the atmosphere, sodium hydroxide is expected to exist as a particulate based upon the low vapor pressure expected for an ionic compound. Sodium hydroxide reacts with carbon dioxide to form sodium carbonate. Wet deposition in rain, snow, or fog is expected to be the dominant fate process in the atmosphere based upon sodium hydroxide's high water solubility.

CHEMICAL SUMMARY FOR SODIUM HYPOPHOSPHITE AND SODIUM HYPOPHOSPHITE MONOHYDRATE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of sodium hypophosphite and its monohydrate are summarized in Tables 1 and 2, respectively.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM
HYPOPHOSPHITE

Characteristic/Property	Data	Reference
CAS No.	7681-53-0	CAS (1998)
Common Synonyms	Phosphinic acid, sodium salt	Budavari et al. (1996)
Molecular Formula	H ₂ NaO ₂ P	Budavari et al. (1996)
Chemical Structure	NaH ₂ PO ₂	Budavari et al. (1996)
Physical State	colorless, pearly, crystalline plates or white granular powder	Lewis (1993)
Molecular Weight	87.98	Budavari et al. (1996)
Melting Point	no data	
Boiling Point	decomposes	Dean (1985)
Water Solubility	approximately 500 g/L ¹	Estimated
Density	no data	
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	Estimated
Log Kow	no data; expected to be <1	Estimated
Vapor Pressure	no data; expected to be < 10 ⁻⁶ mm Hg	Estimated
Reactivity	Explosion risk when mixed with strong oxidizing agents.	Lewis (1993)
Flammability	no data	
Flash Point	no data	
Dissociation Constant	2.1 (phosphinic acid)	Fee et al. (1996)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ Estimated from a reported solubility of 100 parts in 100 parts at 25 °C for the monohydrate (Dean 1985).

TABLE 2. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SODIUM HYPOPHOSPHITE MONOHYDRATE

Characteristic/Property	Data	Reference
CAS No.	10039-56-2	CAS (1998)
Molecular Formula	NaPH ₂ O ₂ ·H ₂ O	Dean (1985)
Chemical Structure	NaPH ₂ O ₂ ·H ₂ O	Dean (1985)
Physical State	white, monoclinic	Dean (1985)
Molecular Weight	105.99	Dean (1985)
Melting Point	loses water at 200°C	Dean (1985)
Boiling Point	decomposes	Dean (1985)
Water Solubility	approximately 500 g/L ¹	Estimated
Density	no data	
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	Estimated
Log Kow	no data; expected to be <1	Estimated
Vapor Pressure	no data; expected to be < 10 ⁻⁶ mm Hg	Estimated
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	2.1 (phosphinic acid)	Fee et al. (1996)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ Estimated from a reported solubility of 100 parts in 100 parts at 25°C (Dean 1985).

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Almost all sodium salts are highly dissociated in natural waters (Bodek et al., 1988). Therefore, if sodium hypophosphite is released into water, it is expected to initially hydrate to form the monohydrate then dissociate into hypophosphite (H₂PO₂⁻) and sodium (Na⁺) ions. The pKa of phosphinic acid indicates that hypophosphite will exist mainly in the dissociated state in the environment. The dissociation of sodium hypophosphite into its component ions indicates sodium hypophosphite will not volatilize from water surfaces or bioconcentrate in aquatic organisms. The sodium ion is expected to exist predominately as the free ion in most natural waters (Bodek et al., 1988). Ion exchange processes with suspended solids and sediment in the water column are expected to remove ionic sodium from solution; however, sodium binds weakly to ion exchange sites and is expected to be displaced by other cations present in natural waters (Bodek et al., 1988). No information specifically regarding the environmental fate of the phosphinic acid or hypophosphite ion in water was located in the available literature. Phosphinic acid and its salts are strong reducing agents; they are oxidized to phosphonic acid or phosphonate (H₃PO₃ or HPO₃²⁻) (Fee et al., 1996). It is unclear how rapidly this process will occur in the environment.

B. Atmospheric Fate

If sodium hypophosphite or its monohydrate are released to the atmosphere, it is expected to exist as a particulate based upon the low vapor pressure expected for this compound. Particulates of the unhydrated salt may also hydrate when exposed to moisture in the atmosphere to form the monohydrate. Wet deposition of sodium hypophosphite in

rain, snow, or fog is expected to be the dominant fate process in the atmosphere (Arimoto, 1989) based upon its high water solubility (Betterman et al., 1991).

C. Terrestrial Fate

If sodium hypophosphite is released to soil, it is expected to initially hydrate to form the monohydrate then dissociate into its component ions in moist soils. The pKa of phosphinic acid indicates that it will exist mainly in the dissociated state in the environment. The low vapor pressure and low Henry's Law constant expected for an ionic salt indicates that neither sodium hypophosphite nor its hydrate will volatilize from either moist or dry soil surfaces. In soil, ion exchange processes are important in retarding the mobility of sodium ions, however they may be replaced by other soil cations since the sodium ion is held weakly by soils (Evans, 1989). No information specifically regarding the environmental fate of the phosphinic acid or hypophosphite ion in soils was located in the available literature. Phosphinic acid and its salts are a strong reducing agents; they are oxidized to phosphonic acid or phosphonate (H_3PO_3 or HPO_3^{2-}) (Fee et al., 1996). It is unclear how rapidly this process will occur in the environment.

D. Summary

If released into water, sodium hypophosphite and its hydrate are expected to dissociate into sodium and hypophosphite ions. The dissociation of sodium hypophosphite into its component ions indicates that it will not volatilize from water surfaces or bioconcentrate in aquatic organisms. The sodium ion is expected to participate in ion exchange reactions with charged surfaces of suspended sediments and sediment in the water column. If released into soil, sodium hypophosphite and its hydrate are expected to dissociate into its component ions in moist soils. As a result, sodium hypophosphite is not expected to volatilize from moist soil surfaces. The mobility of sodium ions will be retarded by ion exchange processes with charged surfaces of soil particles. However, since the sodium ion is held weakly by ion exchange processes, it may leach into groundwater. Phosphinic acid and its salts are a strong reducing agents; they are oxidized to phosphonic acid or phosphonate (H_3PO_3 or HPO_3^{2-}). It is unclear how rapidly this process will occur in either soil or water environments. The low vapor pressure expected for an ionic salt indicates that neither sodium hypophosphite nor its monohydrate are expected to volatilize from dry soil surfaces. If released to the atmosphere, the low vapor pressure expected for an ionic salt indicates that sodium hypophosphite will exist as a particulate in the ambient atmosphere. Wet and dry deposition will be the dominant fate process in the atmosphere.

CHEMICAL SUMMARY FOR STANNOUS METHANESULFONIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of stannous methanesulfonic acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF STANNOUS METHANESULFONIC ACID

Characteristic/Property	Data	Reference
CAS No.	53408-94-9	CAS (1998)
Molecular Formula	C ₂ H ₆ O ₆ S ₂ Sn	SRC (1998)
Chemical Structure	[H ₃ CS(O)(O)O]Sn[OS(O)(O)CH ₃]	SRC (1998)
Physical State	no data	
Molecular Weight	310.89	SRC (1998)
Melting Point	no data	
Boiling Point	no data	
Water Solubility	no data	
Density	no data	
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	Estimated
Log Kow	no data; expected to be <1	Estimated
Vapor Pressure	no data; expected to be <10 ⁻⁶ mm Hg at 25°C	Estimated
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If stannous methanesulfonic acid is released into water, it is expected to dissociate into tin (Sn²⁺) and methanesulfonate (CH₃SO₃⁻) ions. The dissociation of stannous methanesulfonic acid into its component ions indicates that stannous methanesulfonic acid is not expected to bioconcentrate in aquatic organisms or volatilize from water surfaces. Ionic tin may adsorb to charged surfaces of suspended sediments and humic materials in the water column (Evans, 1989). Methanesulfonic acid has a pKa of -1.86 (Serjeant and Dempsey, 1979 as cited in PHYSPROP, 1998) indicating that it will exist in the ionized at pH values typically encountered in the environment. Therefore, volatilization of methanesulfonate from water surfaces is not expected to be an important fate process. Methanesulfonate ions may adsorb to charged surfaces of suspended solids and sediment in the water column,

although the importance of this process in the environment is not known. Limited data indicate that biodegradation of methanesulfonate may be an important fate process (HSDB, 1998). An estimated BCF of 3 for methanesulfonic acid (Meylan et al., 1997) suggests the potential for bioconcentration in aquatic organisms is low (Franke et al., 1994).

B. Atmospheric Fate

If stannous methanesulfonic acid is released to the atmosphere, the low vapor pressure expected for an ionic salt indicates that it will exist as a particulate. Dry deposition of stannous methanesulfonic acid is expected to be the dominant fate process in the atmosphere (Arimoto, 1989). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). Wet deposition of stannous methanesulfonic acid may occur (Arimoto, 1989) in rain, snow, or fog.

C. Terrestrial Fate

If stannous methanesulfonic acid is released to soil, it is expected to dissociate into its component ions in moist soils. The dissociation of stannous methanesulfonic acid into its component ions in moist soils indicates that stannous methanesulfonic acid is not expected to volatilize from moist soil surfaces. The low vapor pressure expected for an ionic salt indicates that stannous methanesulfonic acid is not expected to volatilize from dry soil surfaces. Ionic tin may adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces (Evans, 1989) and therefore its rate of migration through soil may be slow. Methanesulfonic acid has a pKa of -1.86 (Serjeant and Dempsey, 1979 as cited in PHYSPROP, 1998) indicating it will exist in the ionized form in moist soils in the environment. Therefore, volatilization of methanesulfonate from moist soil surfaces will not occur. Methanesulfonate ions may adsorb to charged surfaces of soil particles, however the importance of this process in the environment is unknown. Limited data indicate that biodegradation of methanesulfonate may be an important fate process (HSDB, 1998).

D. Summary

If released into water, stannous methanesulfonic acid is expected to dissociate into tin and methanesulfonate ions. The dissociation of stannous methane sulfonic acid into its component ions indicates that stannous methanesulfonic acid is not expected to bioconcentrate in aquatic organisms nor volatilize from water surfaces. Ionic tin may adsorb to charged surfaces of suspended sediments and humic materials in the water column. Methanesulfonate ions may adsorb to charged surfaces of suspended sediments and humic materials in the water column, however the importance of this process in the environment is unknown. If released to soil, stannous methanesulfonic acid is expected to dissociate into its component ions in moist soils. The dissociation of stannous methanesulfonic acid into its component ions in moist soils indicates that volatilization from soil surfaces is not expected to be an important fate process. Ionic tin may adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces and therefore its rate of migration through soil may be slow. Methanesulfonate ions may adsorb to charged surfaces of soil particles, however the importance of this process in the environment is unknown. The low vapor pressure expected for an ionic salt indicates that stannous methanesulfonic acid is not expected to volatilize from dry soil surfaces. Limited data indicate that biodegradation of methanesulfonate may be an important fate process. If released to the atmosphere, stannous methanesulfonic acid is expected to exist as a particulate in the ambient atmosphere based upon the low vapor pressure expected for an ionic salt. Wet and dry deposition will be the dominant fate process in the atmosphere. The rate of dry deposition will depend on the prevailing winds and particle size.

CHEMICAL SUMMARY FOR SULFURIC ACID

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of sulfuric acid are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF SULFURIC ACID

Characteristic/Property	Data	Reference
CAS No.	7664-93-9	CAS (1998)
Common Synonyms	Battery acid	Weiss (1986)
Molecular Formula	H ₂ O ₄ S	Budavari et al. (1996)
Chemical Structure	H ₂ SO ₄	Budavari et al. (1996)
Physical State	colorless oily liquid	Lide (1995)
Molecular Weight	98.080	Lide (1995)
Melting Point	10.31 °C	Lide (1995)
Boiling Point	337 °C	Lide (1995)
Water Solubility	1000 g/L at 25° C	Gunther et al. (1968) as cited in PHYSPROP (1998)
Density	1.8 g/cm ³	Lide (1995)
Vapor Density (air = 1)	not pertinent	Weiss (1986)
Koc	no data; expected to be <10	Estimated
Log Kow	no data; expected to be <1	Estimated
Vapor Pressure	5.98X10 ⁻⁵ mm Hg at 25°C	Daubert and Danner (1987)
Reactivity	very reactive, dissolves most metals; concentrated acid oxidizes, dehydrates, or sulfonates most organic compounds, often causes charring.	Lewis (1993)
Flammability	not flammable	Weiss (1986)
Flash Point	not flammable	Weiss (1986)
Dissociation Constant	pK _{a1} = -3.00, pK _{a2} = 1.99	Bodek et al. (1988)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	Estimated
Fish Bioconcentration Constant	no data	
Odor Threshold	greater than 1 mg/m ³	Weiss (1986)

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If sulfuric acid is released into the water column at low concentrations, a pK_{a1} of -3.00 (Bodek et al., 1988) indicates sulfuric acid will dissociate into bisulfate (HSO₄⁻) and hydrogen (H⁺) ions. In virtually all natural waters, the bisulfate ion will also dissociate into sulfate (SO₄²⁻) and hydrogen ions based upon a pK_a of 1.99 (Bodek et al., 1988). Sulfuric acid will form salts with basic components in water. The dissociation of sulfuric acid into its component ions indicates that sulfuric acid is not expected to volatilize from water surfaces or bioconcentrate in aquatic

organisms. Sulfate ions may participate in oxidation-reduction reactions or react with cations present in the water column to form soluble complexes or insoluble precipitates (Bodek et al., 1988). Sulfate-reducing microorganisms are important mediators in redox reactions involving this ion (Bodek et al., 1988). Large releases of the concentrated acid into water, such as may result from a spill, will result in a lowering of the pH (Bodek et al., 1988).

B. Atmospheric Fate

If sulfuric acid is released to the atmosphere, its vapor pressure (Daubert and Danner, 1987) indicates it will exist as a particulate in the ambient atmosphere. Wet deposition of sulfuric acid in rain, snow, or fog is expected to be the dominant fate process in the atmosphere (Arimoto, 1989) based upon its high water solubility (Gunther et al., 1968 as cited in PHYSPROP, 1998). In the atmosphere, SO_2 is oxidized to sulfuric acid (Graedel et al., 1986).

C. Terrestrial Fate

If sulfuric acid is released to soil, it will dissociate into sulfate and hydrogen ions in moist soils and will form salts with basic soil components. The dissociation of sulfuric acid into its component ions indicates that volatilization from moist soil surfaces is not expected to occur. Sulfate is generally weakly retained by soils (Bodek et al., 1988) and therefore it may leach into groundwater. Adsorption of the sulfate ion may be important in humic soils containing Al and Fe oxides (Bodek et al., 1988). Sulfuric acid's vapor pressure (Daubert and Danner, 1987) indicates that volatilization from dry soil surfaces is not expected to be an important fate process.

D. Summary

If released into water, sulfuric acid will dissociate into sulfate (SO_4^{2-}) and hydrogen (H^+) ions. Therefore, sulfuric acid is not expected to adsorb to suspended solids or sediment in the water column, bioconcentrate in aquatic organisms, nor volatilize from water surfaces. Sulfate ions may participate in redox reactions or react with cations present in the water column. Sulfate-reducing microorganisms have been identified as important mediators in redox reactions involving the sulfate ion. Sulfuric acid will form salts with basic components in water. If released to soil, sulfuric acid is expected to dissociate into its component ions in moist soils and will form salts with basic soil components. The dissociation of sulfuric acid into its component ions indicates that volatilization from moist soil surfaces is not expected to be an important fate process. In general, sulfate is weakly retained by soils and therefore it may leach into groundwater. Adsorption of the sulfate ion may be important in soils with high organic matter content or soils containing Al and Fe oxides. Sulfuric acid's vapor pressure indicates that volatilization from dry soil surfaces is not expected to occur. If released to the atmosphere, sulfuric acid is expected to exist as a particulate. Sulfuric acid is expected to be physically removed from the atmosphere by wet deposition based upon its high water solubility.

CHEMICAL SUMMARY FOR THIOUREA

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of thiourea are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF THIOUREA

Characteristic/Property	Data	Reference
CAS No.	62-56-6	CAS (1998)
Common Synonyms	Thiocarbamide	Lide (1995)
Common Synonyms	Urea, 2-thio	Howard and Neal (1992)
Molecular Formula	CH ₄ N ₂ S	Lide (1995)
Chemical Structure	H ₂ NC(=S)NH ₂	Budavari et al. (1996)
Physical State	crystals	Budavari et al. (1996)
Molecular Weight	76.12	Lide (1995)
Melting Point	182 °C	Lide (1995)
Boiling Point	no data	
Water Solubility	201 g/L at 20 °C	Yalkowsky and Dannenfelser (1992)
Density	1.405 g/cm ³ at 25 °C	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; estimated to be 2.8	Meylan et al. (1992)
Log Kow	-1.02	Hansch et al. (1995)
Vapor Pressure	3.11X10 ⁻⁴ mm Hg at 25 °C (extrapolated)	Daubert and Danner (1992)
Reactivity	no data	
Flammability	no data	
Flash Point	no data	
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; estimated to be 1.6X10 ⁻⁷	Meylan and Howard (1991)
Fish Bioconcentration Constant	<0.2 to <2 in carp	Chemicals Inspection and Testing Institute (1992)
Odor Threshold	no data	

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If thiourea is released into water, an estimated Koc value of 2.8 (Meylan et al., 1992) indicates that thiourea is not expected to adsorb to suspended solids and sediment in the water column (Swann et al., 1983). According to a classification scheme (Franke et al., 1994), BCFs of <0.2 and <2 in carp (Chemicals Inspection and Testing Institute, 1992) indicate that bioconcentration in aquatic organisms is low. An estimated Henry's Law constant of 1.6X10⁻⁷ atm m³/mole at 25 °C (Meylan and Howard, 1991) indicates that thiourea is expected to be essentially nonvolatile

from water surfaces (Lyman et al., 1990). Thiourea has been demonstrated to be resistant to biodegradation in a variety of standard biodegradation tests (HSDB, 1998). Thiourea reached 2.6% of its theoretical biological oxygen demand over 2 weeks in the Japanese MITI test using an activated sludge seed and an initial chemical concentration of 30 mg/L (Chemicals Inspection and Testing Institute, 1992). In the OECD-screening test, 3% degradation was observed (Schmidt-Bleek et al., 1982 as cited in HSDB, 1998) and 17% CO₂ evolution was measured in a 5-day German GSF Biodegradation Test (Rott et al., 1982 as cited in HSDB, 1998). Thiourea is stable to hydrolysis at environmental pHs (Schmidt-Bleek et al., 1982 as cited in HSDB, 1998).

B. Atmospheric Fate

If thiourea is released to the atmosphere, an extrapolated vapor pressure of 3.11×10^{-4} mm Hg at 25°C (Daubert and Danner, 1992) indicates that thiourea will exist as a gas in the ambient atmosphere (Bidleman, 1988). The rate constant for the gas-phase reaction of urea with photochemically-produced hydroxyl radicals has been estimated to be 4.2×10^{-11} cm³/molecule-sec at 25°C (Meylan and Howard, 1993); this corresponds to a half-life of 9.2 hours.

C. Terrestrial Fate

If thiourea is released to soil, an estimated Koc value of 2.8 (Meylan et al., 1992) indicates that thiourea is expected to have very high mobility in soils (Swann et al., 1983). Thiourea is not expected to volatilize from moist soil surfaces (Lyman et al., 1990) based upon its estimated Henry's Law constant (Meylan and Howard, 1991) or from dry soils based on its vapor pressure. Biodegradation of thiourea by soil microorganisms may be an important fate process, although microflora activity may be suppressed for extended periods of time by high concentrations of this compound (HSDB, 1998). Degradation of thiourea was also observed in sterilized soils (Kolyada, 1969 as cited in HSDB, 1998) indicating that abiotic degradation may be an important fate process.

D. Summary

If released into water, thiourea is not expected to be adsorb to suspended solids and sediment in the water column. Bioconcentration in aquatic organisms and volatilization from water surfaces are not expected to be important fate processes. Several biodegradation tests indicate that thiourea may be resistant to biodegradation. Thiourea is stable to hydrolysis at environmental pHs. If released to the atmosphere, thiourea is expected to exist as a gas in the ambient atmosphere based upon its extrapolated vapor pressure. Gas-phase thiourea is expected to be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air has been estimated to be 9.2 hours. If released to soil, thiourea is expected to have very high mobility and therefore may leach into groundwater. Volatilization from moist or dry soil surfaces is not expected to be an important fate process. Biotic and abiotic degradation of thiourea may be important fate processes, however, no rates were available for these processes. High concentrations of thiourea may suppress the activity of soil microorganisms for extended periods of time.

CHEMICAL SUMMARY FOR TIN

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources. The search identified sources of information for Tin.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of Tin are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF TIN

Characteristic/Property	Data	Reference
CAS No.	7440-31-5	Howard and Neal (1992)
Common Synonyms	Tin white	Weast (1983)
Molecular Formula	Sn	Howard and Neal (1992)
Chemical Structure		
Physical State	Metal	Budavari et al. (1996)
Molecular Weight	118.69	Budavari et al. (1996)
Melting Point	231.9°C	Weast (1983)
Boiling Point	2260°C	Weast (1983)
Water Solubility	Insoluble	Weast (1983)
Density	7.31g/mL	Weast (1983)
Vapor Density (air = 1)	no data	
Koc	no data	
Log Kow	no data	
Vapor Pressure	no data	
Reactivity	Flammable solid	Budavari et al. (1996)
Flammability	no data	
Flash Point	no data	
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data	
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

CHEMICAL SUMMARY FOR TIN CHLORIDE

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of tin chloride are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF TIN CHLORIDE

Characteristic/Property	Data	Reference
CAS No.	7772-99-8	CAS (1998)
Common Synonyms	Tin (II) chloride	Lide (1995)
Common Synonyms	Stannous chloride	Lewis (1993)
Molecular Formula	Cl ₂ Sn	Sax (1984)
Chemical Structure	SnCl ₂	Lide (1995)
Physical State	white orthorhombic crystals	Lide (1995)
Molecular Weight	189.615	Lide (1995)
Melting Point	247 °C	Lide (1995)
Boiling Point	623 °C	Lide (1995)
Water Solubility	approximately 600 g/L ¹	Estimated
Density	3.90 g/cm ³	Lide (1995)
Vapor Density (air = 1)	no data	
Koc	no data; expected to be <10	SRC (1998)
Log Kow	no data; expected to be <1	SRC (1998)
Vapor Pressure	no data; expected to be < 10 ⁻⁶ mm Hg	SRC (1998)
Reactivity	violent reactions with BrF ₃ , CaC ₂ , ethylene oxide, hydrazine hydrate, nitrates, K, Na, H ₂ O ₂	Sax (1984)
Flammability	no data	
Flash Point	no data	
Dissociation Constant	expected to dissociate into Sn ²⁺ and Cl ⁻	SRC (1998)
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; expected to be <1X10 ⁻⁸	SRC (1998)
Fish Bioconcentration Constant	no data	
Odor Threshold	no data	

¹ Estimated from a reported solubility of 84 parts in 100 parts water (Dean, 1985).

II. ENVIRONMENTAL FATE

A. Aquatic Fate

Water hydrolyzes tin halides (Cotton and Wilkinson, 1980). Therefore, if tin chloride is released into water, it is expected to dissociate into tin (Sn²⁺) and chloride (Cl⁻) ions. In waters containing excess chloride ion, tin chloride is expected to dissolve, yielding SnCl₃⁻ (Cotton and Wilkinson, 1980). As a result, tin chloride is not expected to volatilize from water surfaces or bioconcentrate in aquatic organisms. Ionic tin may adsorb to charged surfaces of

suspended sediments and humic materials in the water column (Evans, 1989). The chloride ion may complex with heavy metals, thereby increasing their solubility (Bodek et al., 1988). Adsorption of the chloride ion to suspended solids and sediment in the water column is not expected to be an important fate process.

B. Atmospheric Fate

If tin chloride is released to the atmosphere, the low vapor pressure expected for an ionic salt indicates that it will exist as a particulate. Dry deposition of tin chloride is expected to be the dominant fate process in the atmosphere (Arimoto, 1989). The rate of dry deposition will depend on the prevailing winds and particle size (Bodek et al., 1988). Tin chloride is expected to undergo wet deposition (Arimoto, 1989) in rain, snow, or fog due to its high water solubility (Dean, 1985).

C. Terrestrial Fate

Water hydrolyzes tin halides (Cotton and Wilkinson, 1980). Therefore, if tin chloride is released to soil, it is expected to dissociate into its component ions in moist soils. Ionic tin may adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces (Evans, 1989) and therefore its rate of migration through soil may be slow. The dissociation of tin chloride into its component ions in moist soils indicates that tin chloride is not expected to volatilize from moist soil surfaces. The low vapor pressure expected for an ionic salt indicates that tin chloride is not expected to volatilize from dry soil surfaces. Chloride is extremely mobile in soils (Bodek et al., 1988). The chloride ion may complex with heavy metals, thereby increasing their solubility (Bodek et al., 1988) and potential for leaching into groundwater.

D. Summary

If released into water, tin chloride is expected to dissociate into tin and chloride ions. The dissociation of tin chloride into its component ions indicates that tin chloride is not expected to volatilize from water surfaces or bioconcentration in aquatic organisms. Ionic tin may adsorb to charged surfaces of suspended sediments and humic materials in the water column. The chloride ion may complex with heavy metals, thereby increasing their solubility. Adsorption of the chloride ion to suspended solids and sediment in the water column is not expected to be an important fate process. If released to soil, tin chloride is expected to dissociate into its component ions in moist soils. The dissociation of tin chloride into its component ions in moist soils indicates that tin chloride is not expected to volatilize from moist soil surfaces. The low vapor pressure expected for an ionic salt indicates that tin chloride is not expected to volatilize from dry soil surfaces. Ionic tin may adsorb to charged surfaces of soil particles or form inner sphere complexes with variable-charge soil surfaces and therefore its rate of migration through soil may be slow. The chloride ion is extremely mobile in soils; it may complex heavy metals, thereby increasing their solubility and the potential to leach into groundwater. If released to the atmosphere, tin chloride is expected to exist as a particulate in the ambient atmosphere based upon the low vapor pressure expected for an ionic salt. Wet and dry deposition will be the dominant fate process in the atmosphere. The rate of dry deposition will depend on the prevailing winds and particle size.

CHEMICAL SUMMARY FOR UREA

This summary is based on information retrieved from a systematic search limited to secondary sources. The only exception is summaries of studies from unpublished TSCA submissions that may have been included. These sources include online databases, unpublished EPA information, government publications, review documents, and standard reference materials. No attempt has been made to verify information in these databases and secondary sources.

I. CHEMICAL IDENTITY AND PHYSICAL/CHEMICAL PROPERTIES

The chemical identity and physical/chemical properties of urea are summarized in Table 1.

TABLE 1. CHEMICAL IDENTITY AND CHEMICAL/PHYSICAL PROPERTIES OF UREA

Characteristic/Property	Data	Reference
CAS No.	57-13-6	CAS (1998)
Common Synonyms	Carbamide	Lide (1995)
Common Synonyms	Carbonyldiamide	Budavari et al. (1996)
Molecular Formula	CH ₄ N ₂ O	Lide (1995)
Chemical Structure	H ₂ NC(=O)NH ₂	Budavari et al. (1996)
Physical State	Tetragonal prisms	Budavari et al. (1996)
Molecular Weight	60.06	Lide (1995)
Melting Point	132.7 °C	Lide (1995)
Boiling Point	decomposes	Lide (1995)
Water Solubility	545 g/L at 25 °C	Yalkowsky and Dannenfelser (1992)
Density	1.3230 g/cm ³ at 20 °C	Lide (1995)
Vapor Density (air = 1)	not pertinent	Weiss (1986)
Koc	8	Hance (1965) as cited in HSDB (1998)
Log Kow	-2.11	Hansch et al. (1995)
Vapor Pressure	1.2X10 ⁻⁵ mm Hg at 25 °C (extrapolated)	Jones (1960) as cited in PHYSPROP (1998)
Reactivity	no reaction with water or common materials	Weiss (1986)
Flammability	not flammable	Weiss (1986)
Flash Point	not flammable	Weiss (1986)
Dissociation Constant	no data	
Molecular Diffusivity Constant	no data	
Air Diffusivity Constant	no data	
Henry's Law Constant	no data; estimated to be less than 1X10 ⁻⁸	PHYSPROP (1998)
Fish Bioconcentration Constant	<10	Freitag et al. (1985) as cited in HSDB (1998)
Odor Threshold	not pertinent	Weiss (1986)

II. ENVIRONMENTAL FATE

A. Aquatic Fate

If urea is released into water, a Koc value of 8 (Hance, 1965 as cited in HSDB, 1998) indicates that urea is not expected to adsorb to suspended solids and sediment in the water column (Swann et al., 1983). According to a classification scheme (Franke et al., 1994), a BCF of <10 in golden ide (Freitag et al., 1985 as cited in HSDB, 1998) indicates that bioconcentration in aquatic organisms is low. An estimated Henry's Law constant of <1X10⁻⁸ atm m³/mole at 25 °C (PHYSPROP, 1998) indicates that urea is expected to be essentially nonvolatile from water

surfaces (Lyman et al., 1990). In natural waters, biodegradation of urea is expected to be an important fate process; ammonia and carbon dioxide have been identified as degradation products (HSDB, 1998). The rate of biodegradation is expected to decrease with decreasing temperatures; at 8°C, negligible degradation was observed after incubation in river water for 14 days, while at 20°C complete degradation was observed after 4 to 6 days incubation (Evans and Patterson, 1973 as cited in HSDB, 1998). The presence of naturally-occurring phytoplankton in water is expected to increase the rate of biodegradation (HSDB, 1998). Urea is used as an agricultural fertilizer (Lewis, 1993) and will be taken up by plants as a source of nitrogen. Abiotic hydrolysis of urea occurs slowly yielding ammonium carbamate (HSDB, 1998). At 5°C, 0.35% of urea hydrolyzed during a 10-day test period in demineralized/distilled water (Atkinson, 1971 as cited in HSDB, 1998).

B. Atmospheric Fate

If urea is released to the atmosphere, a vapor pressure of 1.2×10^{-5} mm Hg at 25°C (Jones, 1960 as cited in PHYSPROP, 1998) indicates that urea will exist as both a particulate and a gas in the ambient atmosphere (Bidleman, 1988). The rate constant for the gas-phase reaction of urea with photochemically-produced hydroxyl radicals has been estimated to be 2.0×10^{-12} cm³/molecule-sec at 25°C (Meylan and Howard, 1993); this corresponds to a half-life of 8.0 days. Particulate-phase urea is expected to be physically removed from the atmosphere by wet and dry deposition (Arimoto, 1989).

C. Terrestrial Fate

If urea is released to soil, it is expected to hydrolyze to ammonia through soil urease activity (HSDB, 1998). The rate of hydrolysis can range from 24 hours to weeks depending upon soil type, moisture content, and urea formulation (Malhi and Nyborg, 1979 as cited in HSDB, 1998). Urea is used as an agricultural fertilizer (Lewis, 1993) and will be taken up by plants as a source of nitrogen. While no specific studies were identified in the literature, it is anticipated that urea will biodegrade rapidly in soil as has been reported in water. A Koc value of 8 (Hance, 1965 as cited in HSDB, 1998) indicates that urea is expected to have very high mobility in soils (Swann et al., 1983). Urea is not expected to volatilize from soil surfaces based upon its vapor pressure and estimated Henry's Law constant.

D. Summary

If released into water, urea is expected to be biodegraded yielding ammonia and carbon dioxide. Biodegradation is expected to be more rapid in waters containing phytoplankton and during summer months when warmer water temperatures prevail. Urea will be taken up by plants and used as a source of nitrogen. Bioconcentration in aquatic organisms, adsorption to suspended solids and sediment in the water column, and volatilization from water surfaces are not expected to be important fate processes. If released to the atmosphere, urea is expected to exist as both a particulate and as a gas based upon its vapor pressure. Gas-phase urea is expected to be degraded in the atmosphere by reaction with photochemically-produced hydroxyl radicals; the half-life for this reaction in air has been estimated to be 8.0 days. Particulate-phase urea is expected to be physically removed from the atmosphere by wet and dry deposition. The rate of dry deposition will depend upon particle size and prevailing wind patterns. If released to soil, urea is expected to hydrolyze to ammonia through the activity of soil urease as well as biodegrade as is the case in water. The rate of hydrolysis can range from 24 hours to weeks depending upon soil type, moisture content, and urea formulation. Urea is used as an agricultural fertilizer as a source of nitrogen. Urea is expected to have very high mobility in soils and therefore may leach into groundwater. Volatilization from moist and dry soil surfaces is not expected to be an important fate process.

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